



HEADQUARTERS
U.S. ARMY ARMAMENT,
MUNITIONS AND CHEMICAL COMMAND

FINAL REPORT

DEVELOPMENT OF
METHODOLOGY AND TECHNOLOGY
FOR
IDENTIFYING AND QUANTIFYING
EMISSION PRODUCTS
FROM
OPEN BURNING AND OPEN DETONATION
THERMAL TREATMENT METHODS.

FIELD TEST SERIES A, B, AND C

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VOLUME 1
TEST SUMMARY

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based on the conversion of the carbon in the explosive material to CO₂. The semivolatiles in the soil were identified, quantified and a comparison made between background levels and after detonations levels. Similarity in analyte detected and the levels of analytes measured for TNT, RDX, explosive D, and composition B lead to the conclusion that OB/OD can be an effective means of treatment. Based on TNT the BB EF are comparable to field EF. The propellant burns all resulted in extremely efficient conversion of material carbon into CO₂ >99 percent.

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FOREWORD

A test planning directive to conduct the OB/OD test in support of U.S. Army Armament, Munitions and Chemical Command (AMCCOM) was issued by U.S. Army Test and Evaluation Command (TECOM) on 28 April 1988¹. A Technical Steering Committee Symposium was convened in July 1988. The requirement for identifying and quantifying emissions from the open detonation of explosives and open burning of propellants was discussed in detail by authorities from throughout the military, academic, and commercial communities. Conclusions and recommendations developed during the symposium are reported in proceedings of the symposium².

A series of TNT detonations and propellant burns were characterized in a BangBox (chamber) in December 1988 and January 1989 for the purpose of developing methodology and technology for large scale detonations and burns in the field. The BangBox test is reported in a three volume set. The report covers the details of the methods and technology development and would be useful for those desiring more detail on such things as the carbon balance method, the emission factors from a nonhomogeneous and homogeneous detonation or burn cloud, the samplers selected for future use in the fixed wing aircraft, and the techniques used in extracting and assaying samples.

The field tests took place in 1989 and 1990 and are reported in three volumes.

Volume 1. A summary which describes the planning phase, the conduct of trials, sample analyses and results, and the conclusions and recommendations. It is useful for those who need only a quick review (executive summary) and those who need a detailed description of the conduct and results of the Field Tests Phases A, B, and C.

Volume 2, Part A. A stand-alone document which covers the quality assurance and quality control procedures, the blind spiking of samples, the on site challenges of equipment and

¹Letter, AMSTE-TA-F, Headquarters, U.S. Army Test and Evaluation Command, Aberdeen Proving Ground, Maryland, 20 April 1988, subject: Test Planning Directive for Special Study of Open Burning/Open Detonation (OB/OD), Phase II, TECOM Project No 2-CO-210-000-017.

²*Proceedings of the Technical Steering Committee Symposium 6-8 July 1988*, Headquarters, United States Army Armament, Munitions and Chemical Command, Rock Island, Illinois, August 1991.

personnel, the conclusions, and the recommendations.

Volume 2, Part B. The quality assurance (QA) program plan which was developed specifically to support phase "C" field testing. While directed to phase "C" testing, it also represents the procedures and techniques and QA philosophies which were used during OB/OD field testing phases "A" and "B" and is based on experience gained during these two earlier field tests.

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ABSTRACT

The development, testing, and evaluation of a U.S. Environmental Protection Agency (Office of Solid Waste/Atmospheric Research and Exposure Assessment Laboratory) validated and accepted method for the characterization of emissions from open burning (OB) and open detonation (OD) thermal treatment operations is presented. The methodology utilizes an innovative carbon balance technique to calculate accurate emission factors (Efs) of combustion products in diffusing clouds and a combination of supercritical fluid chromatography (SFC), gas chromatography (GC), and mass spectrometry (MS) to detect and quantify potential air and soil contaminants. These methods were used to achieve maximum sensitivity/identification of volatiles and semivolatile organic compounds. The SFC-MS was able to measure the thermally labile semivolatile organics such as RDX and N-Nitrosodiphenylamine which are subject to breakdown into other compounds with GC-MS. Confirmation of the methodology included closed-chamber tests to check out instrumentation, technology, and analytical procedures proposed for follow-on large-scale open air tests conducted on a fixed wing aircraft flying through the plume. Comparable EFs were obtained from the BangBox (BB) and open air tests for TNT. Because of the similarity in analytes detected, EFs, and concentrations between TNT, composition B, explosive D and RDX, it is reasonable to expect that BB can provide results that will be useful in permit applications.

Materials characterized during the OB/OD study included the explosives TNT, RDX, Explosive D, and Composition B; propellant manufacturing residue; and single-, double-, triple-base, and composite types of propellant. The study and emerging results were briefed as part of a nation-wide EPA-sponsored seminar, on "Incineration and Alternative Treatment of Energetic Compounds to Minimize Effects to Air, Soil and Water Supplies". The seminar was presented to all EPA regions during the period of April-September 1990. The study has confirmed the methodology, technology, and procedures necessary to obtain a portion of data required to obtain permits under provisions of the Resource Conservation and Recovery Act (RCRA), subpart X. Such permitting is required for continuation of all Department of Defense OB/OD operations after 8 November 1992. It is recommended that the methodology and procedures be used in a follow-on program to acquire characterization data on specific munitions, explosives, and propellants that are included in the DoD inventory.

The data obtained will be used to demonstrate that OB/OD units can be operated in a manner so as to meet the environmental performance standards.

EXECUTIVE SUMMARY

Open burning (OB) and open detonation (OD), thermal treatment methods are currently the primary means of demilitarization employed by the Department of Defense (DoD) for the treatment of explosive residue, propellants, and munitions. Increasingly stringent requirements for environmental documentation of potential pollution/contamination from combustion products under such acts as the Clean Air Act, Clean Water Act, and Resource Conservation and Recovery Act (RCRA), resulted in a critical need for technology development to be able to collect data to use as a basis for making informed decisions to determine: (1) the limitations/restrictions of OB/OD thermal treatment methods, (2) the development of alternative treatment methods for munitions/propellants for which OB/OD is not acceptable, and (3) developing and maintaining the most effective, economical, and environmentally safe means of accomplishing required demilitarization/treatment.

The objective of this phase (I) of the OB/OD thermal emission study was to develop and demonstrate the utility of the technologies and methodologies needed to provide the data required for these critical decisions. (See Appendix K)

Under the sponsorship of the Single Manager for Conventional Ammunition within the DoD, a symposium was conducted in July 1988 (Reference 1) to develop planning concepts necessary to address the technical problems associated with an accurate environmental characterization of the OB/OD processes. Authorities from governmental, academic, and private research organizations discussed sampling and sample analysis technologies, data analysis processes, test organization, and preparation of reports that would be acceptable to Federal and State environmental regulatory agencies. Expertise represented included field sampling, instrumentation, field and laboratory analyses, environmental documentation, atmospheric dispersion modeling and sampling, data management, combustion and explosive phenomenology, and quality assurance/quality control. A technical steering committee composed of recognized experts in their respective disciplines was formed under the leadership of the U.S. Army Armament, Munitions and Chemical Command Program Manager.

A list of volatile and semivolatile organic compounds and metals which are potentially hazardous contaminants if they were produced in either the soil or atmosphere from OB/OD processes was developed. A closed chamber (BangBox or BB) test was conducted at Sandia National Laboratories (See Reference 2) to check out instrumentation, technology, methodology, and analytical procedures that were proposed for follow-on large scale field tests to be sampled by a fixed-wing aircraft (FWAC) flying through OB/OD-generated plumes. Representatives of the U.S. Environmental Protection Agency (EPA) (Office of Solid Waste at Washington DC, Region VIII at Denver, CO, and the Quality Assurance Division at Research Triangle Park, NC) served as members of the technical steering committee to provide technical guidance and quality assurance/quality control support during test planning and execution phases, and to review data collection and analytical procedures throughout the entire program. In addition, representatives from the Office of Solid and Hazardous Waste from the State of Utah participated throughout the entire planning and testing period. Real-time and near real-time particulate and gaseous concentration measurements were achieved. These data were correlated with the samples collected on filters and gaseous containers and held for subsequent laboratory analysis. A methodology of using carbon balance to calculate EF factors of combustion products in diffusing clouds was developed. Laboratory analyses of samples utilized innovative supercritical fluid chromatography (in addition to gas chromatography) and mass spectrometry, one of the techniques which attain the lowest possible detection limits for the selected semivolatile analytes.

The BB tests evaluated EF from the open detonation of 2,4,6 trinitrotoluene (TNT), and open burning of a double-base and a composite propellant. The tests confirmed the technologies, methodologies, and analytical procedures employed. These processes were further successfully proven during the conduct of large-scale tests during field tests Phases A, B, and C.

Emissions and residues from propellant manufacturing residue, single- and triple-base, and composite propellants; and TNT, explosive D, RDX and composition B were characterized during the field trials conducted at Dugway Proving Ground (DPG) between June 1989 and September 1990.

Emerging results of the current study were briefed as part of a nationwide EPA-sponsored seminar on "Incineration and Alternative Treatment of Energetic Compounds to Minimize Effects to Air,

Soil, and Water Supplies." The seminar was presented to all EPA regions within the continental United States during the period of April to September 1990. The EPA representatives have accepted the methodology, technology, and procedures as an effective approach to obtain data required for permitting of DoD OB/OD thermal treatment operations.

Results of the study that have direct application to critical decisions on future planning and funding of the DOD demilitarization/treatment program are summarized below:

Comparable EFs were found during BB and field testing for TNT. Additional similarities of the EF, combustion products, and combustion product concentration levels resulting from the OD of TNT, composition B, explosive D, and RDX were observed during large-scale field testing. These two sets of relationships indicate that small-scale BB-type OD tests may be capable of providing the data needed for characterizing large-scale field OD thermal treatment operations and supporting permit applications.

The study also suggests that the bulk explosives and propellants examined during field testing may be treated in an environmentally safe manner by surface OB/OD methods. While these results are encouraging, site-specific testing is needed to provide data to support risk assessments. Only after these risk assessments are completed may a definitive statement be made concerning the effect (if any) OB/OD operations have on human health and the environment.

The advantages of conducting tests in properly designed chambers as opposed to field testing include:

- (1) Costs are reduced and can be more precisely controlled.
- (2) The test environment can be standardized.
- (3) Results may be obtained rapidly.
- (4) Sampling may continue until sufficient quantities of targeted analytes obtained have been collected to meet or exceed minimum quantification level of the analytical methods being used.

(5) Secondary reactions and the decay rate of primary and secondary products of combustion can be studied.

(6) The number of samples necessary for calculating statistically valid EFs (and the uncertainty (imprecision) associated with these EFs) can be acquired under repeatable and well controlled conditions. With this information, a very conservative EF such as the maximum probable EF (upper 95% tolerance level) can be calculated.

(7) Testing delays caused by adverse weather conditions will be minimized.

(8) PEP materials requiring alternative treatment technologies can be rapidly identified.

For those materials that cannot be safely treated by other modes of treatment, the results obtained from chamber testing can be combined with dispersion modelling and health risk assessment information to determine the following:

(1) The type and quantities of pollutants that will be released to the environment from specific PEP items.

(2) Identification of PEP materials for which OB/OD thermal treatment methods are environmentally acceptable.

(3) Those PEP materials that cannot be safely treated in an environmentally safe manner by OB/OD thermal treatment methods, require the development of alternative technologies.

(4) Effective focussing of alternative technologies development.

(5) The design and placement of the monitoring systems that will be required to ensure that the quantities of pollutants released to the environment from permitted OB/OD thermal treatment operations remain at or below the levels specified in the OB/OD permit.

(6) The types of monitoring equipment that must be used and the number of samples of each type that must be taken and the target analytes that must be measured, when chamber studies are inconclusive and an assessment must be made through field testing.

(7) The kinds and quantities of pollutants released from OB/OD thermal treatment operations as the type, quantity, configuration (buried/surface), physical condition (bulk, munition type, old, new), and composition (supplemental oxidants added/not added) is varied.

This combination of testing and modeling will provide the data required to improve/optimize the current OB/OD technology and the environmental sampling and analysis methods employed for monitoring pollutant releases.

The EFs obtained from the BB tests and from the field tests for OD of explosives and OB of propellants is presented in Tables 1, 2, 4, and 5.

Table 1 presents the average EFs for inorganic gases, and volatile organic compounds; Table 2 presents the maximum EFs for semivolatile organic compounds obtained when 225 gram quantities of bulk TNT were detonated in a 1000-m³ BangBox chamber, and results from the trials of three field tests in which 4000 to 10000 lb of bulk TNT, composition B, explosive D, or RDX were detonated on soil at DPG.

The TNT data show that the BB generated EFs are comparable to those obtained in the field. All TNT tests show a very efficient conversion of carbon to CO₂ (>92 percent).

The striking thing about the data in these tables is the very efficient conversion of carbon to CO₂ for all four explosives and the comparable low level of the volatiles and semivolatiles.

A summary of the semivolatile analytes detected in the ejecta soil from the detonations is presented in Table 3. The analytes that were measured after detonation in concentrations greater than those observed in the pretest background are marked with an asterisk. The data shows very few of the analytes detected above background. The parent compound TNT showed elevated levels after the detonations of TNT and composition B.

The results are encouraging because:

- (1) they document the utility of the BB in estimating air emissions in large scale field tests, and
- (2) they indicate that the concentrations of inorganic compounds, volatile organic and semivolatile compounds generated from OD operations may be more predictable than previously supposed.
- (3) they indicate that soil contamination from large-scale high order detonations are very small.

The comparability of EFs obtained for propellants burned in trays at the BB and at DPG parallels the degree of comparability between BB and field detonations. The BB testing of double-base and composite propellants generally yielded EFs that approximated or exceeded those obtained in the field tests, and EFs generated during the OB field testing did not substantially differ from each other. Over 99 percent of the total carbon contained in tested propellants was accounted for in the form of carbon dioxide following the burn event. The semivolatile organics detected were propellant specific, e.g., no semivolatile organic were detected for the M30 (triple-base) propellant burn, but nine semivolatile compounds were detected for the phase B propellant manufacturing residues.

The analyses of samples collected in the fallout and the sputter pans (burns) indicate that the propellants used in this program did not add measurable levels of contamination to the soil beyond 12 m from the propellant burns. The analytes detected and the maximum concentration level of the analyte in the fallout material are shown in Table 6.

The DPG real time volume source dispersion model (RTVSM) was used to estimate ground-level concentrations of selected analytes that would be expected from a 1 metric ton (1000 kg) surface detonation of TNT. Test cases run for typical EFs measured for surface detonated TNT such as CO (EF = 50×10^{-3}), benzene (EF = 0.1×10^{-3}), and benzo[a]pyrene (EF = 0.1×10^{-6}) reveals that maximum ground level peak and 15-minute average concentrations would be indistinguishable from background levels of these pollutants.

The follow on program will obtain emission characterization data for specific munitions and other PEP items in the DoD inventory. Obtaining these critical data and the required permits will eliminate the potential for costly and time consuming litigious actions, and will ensure the continuation of an effective integrated PEP demilitarization/treatment program.

Table 1 Explosive Detonations: Average Emission Factors^a for Inorganic, and Volatile Analytes.

Analyte	TNT RangeBox	TNT Surface Detonations			Phase C Surface Detonations		
		Phase A	Phase B	Phase C	Comp B	^a E _{exp} D	RDX
Percent Carbon Converted to CO ₂	97.1	92.6	94.9	94.1	94.5	92.5	96.6
Carbon dioxide (Theoretical EF ^b)	136	136	136	136	0.921	1.07	0.59
INORGANIC COMPOUNDS							
Carbon dioxide (Empirical EF)	132	126	129	128	0.87	0.99	0.57
Carbon monoxide	4.9 x 10 ⁻³	61 x 10 ⁻³	42 x 10 ⁻³	49 x 10 ⁻³	31 x 10 ⁻³	53 x 10 ⁻³	31 x 10 ⁻³
Nitrogen oxide	11 x 10 ⁻³	0.70 x 10 ⁻³	1.4 x 10 ⁻³	1.4 x 10 ⁻³	0.8 x 10 ⁻³	0.9 x 10 ⁻³	0.9 x 10 ⁻³
Nitrogen dioxide	0.56 x 10 ⁻³	3.6 x 10 ⁻³	1.1 x 10 ⁻³	1.4 x 10 ⁻³	1.0 x 10 ⁻³	1.1 x 10 ⁻³	0.6 x 10 ⁻³
VOLATILE COMPOUNDS							
Methane	0.025 x 10 ⁻³	1.5 x 10 ⁻³	1.2 x 10 ⁻³	1.5 x 10 ⁻³	0.6 x 10 ⁻³	2.4 x 10 ⁻³	0.2 x 10 ⁻³
Total Nonmethane hydrocarbons	0.057 x 10 ⁻³	1.4 x 10 ⁻³	1.9 x 10 ⁻³	2.1 x 10 ⁻³	1.2 x 10 ⁻³	2.0 x 10 ⁻³	1.3 x 10 ⁻³
Benzene	2.4 x 10 ⁻⁴	94 x 10 ⁻⁴	93 x 10 ⁻⁴	100 x 10 ⁻⁴	62 x 10 ⁻⁴	110 x 10 ⁻⁴	69 x 10 ⁻⁴

^aEmission factor—a dimensionless number that, when multiplied by the weight of explosive or propellant material, detonated or burned, results in the weight of analyte expected.

^bTheoretical EF (emission factor) if all carbon is converted to CO₂.

Table 2 Explosive Detonations: Maximum Emission Factors^a for Semivolatile Analytes.

Analyte	TNT Range Box	TNT Surface Detonations			Phase C Surface Detonations		
		Phase A	Phase B	Phase C	Comp B	Exp D	RDX
SEMIVOLATILE COMPOUNDS							
2,4-Dinitrotoluene	170 x 10 ⁻³	150 x 10 ⁻³	8400 x 10 ⁻³	BD ^a	450 x 10 ⁻³	590 x 10 ⁻³	210 x 10 ⁻³
2,6-Dinitrotoluene	140 x 10 ⁻³	19 x 10 ⁻³	7100 x 10 ⁻³	BD	24 x 10 ⁻³	80 x 10 ⁻³	41 x 10 ⁻³
2,4,6-Trinitrotoluene	620 x 10 ⁻³	220 x 10 ⁻³	150 x 10 ⁻³	60 x 10 ⁻³	250 x 10 ⁻³	44 x 10 ⁻³	98 x 10 ⁻³
2-Nitronaphthalene	160 x 10 ⁻³	80 x 10 ⁻³	270 x 10 ⁻³	BD	86 x 10 ⁻³	43 x 10 ⁻³	49 x 10 ⁻³
N-Nitrosodiphenylamine	200 x 10 ⁻³	BD	4.4 x 10 ⁻³	BD	36 x 10 ⁻³	58 x 10 ⁻³	BD
1,3,5-Trinitrobenzene	0.45 x 10 ⁻³	BD	BD	BD	59 x 10 ⁻³	18 x 10 ⁻³	44 x 10 ⁻³
2-Nitrodiphenylamine	NA ^c	BD	NA	BD	72 x 10 ⁻³	58 x 10 ⁻³	34 x 10 ⁻³
1-Nitropyrene	BD	BD	39 x 10 ⁻³	BD	56 x 10 ⁻³	11 x 10 ⁻³	50 x 10 ⁻³
RDX	NA	NA	NA	NA	BD	NA	2100 x 10 ⁻³
Picric acid	NA	NA	NA	NA	NA	50 x 10 ⁻³	NA
Naphthalene	28000 x 10 ⁻³	BD	3700 x 10 ⁻³	2600 x 10 ⁻³	420 x 10 ⁻³	630 x 10 ⁻³	200 x 10 ⁻³
Benz[a]anthracene	BD	2.2 x 10 ⁻³	160 x 10 ⁻³	100 x 10 ⁻³	7.4 x 10 ⁻³	19 x 10 ⁻³	93 x 10 ⁻³
Benzo[a]pyrene	360 x 10 ⁻³	BD	240 x 10 ⁻³	BD	14 x 10 ⁻³	38 x 10 ⁻³	140 x 10 ⁻³
Pyrene	32 x 10 ⁻³	BD	NA	220 x 10 ⁻³	210 x 10 ⁻³	180 x 10 ⁻³	220 x 10 ⁻³
Phenol	9900 x 10 ⁻³	BD	5200 x 10 ⁻³	BD	---	---	---
Dibenzofuran	150 x 10 ⁻³	BD	85 x 10 ⁻³	180 x 10 ⁻³	BD	110 x 10 ⁻³	2000 x 10 ⁻³
Diphenylamine	BD	NA	7.7 x 10 ⁻³	170 x 10 ⁻³	66 x 10 ⁻³	19 x 10 ⁻³	310 x 10 ⁻³

^aEmission factor—a dimensionless number that, when multiplied by the weight of explosive or propellant material, detonated or burned, results in the weight of analyte expected.

^bBD - below detection limit.

^cNA - not a target analyte.

^dPhenol was lost in the extraction of the semivolatile.

Table 3 Explosive Detonations: Semivolatile Analytes Detected and Maximum Recovery in Soil Ejecta (ng/g)^a.

	TNT	Comp B	Exp D	RDX
SEMIVOLATILE COMPOUNDS				
2,4-Dinitrotoluene	8.0	17	1.3	2.0
2,6-Dinitrotoluene	2.3	1.0	0.14	0.90
2,4,6-Trinitrotoluene	360 **	14 *	7.4	0.67
2-Nitronaphthalene	1.8	0.39	0.11	0.90
N-Nitrosodiphenylamine	1.1	0.39	0.090	1.7
1,3,5-Trinitrobenzene	39 *	0.39	0.14	0.77
2-Nitrodiphenylamine	BD ^c	0.60	0.24	0.19
1-Nitropyrene	1.2	0.14	0.12	0.23
RDX	NA ^d	BD	NA	15
Picric acid	NA	NA	BD	NA
Naphthalene	210	13	11	5.3 *
Benz[a]anthracene	11 *	1.9	5.4	2.4
Benzo[a]pyrene	BD	0.53	0.67	0.41
Pyrene	53 *	4.5	5.2 *	5.3 *
Phenol	69 *	---	---	---
Dibenzofuran	18	1.6	1.0	0.95
Diphenylamine	0.79	1.6	0.26	0.48

^aRepresents ng of analyte per g of soil.

^bThe asterisk indicates that the analyte was detected above background level ($P > 0.95$).

^cBD - below detection limit.

^dNA - not a target analyte.

^ePhenol was lost in the extraction of the semivolatile.

Table 4 Propellant Burns: Average Emission Factors^a for Inorganic and Volatile Analytes.

Analyte	BangBox		Phase A Triple Base	Manufacturing Residue		Phase C	
	Double Base	Composite		Phase B	Phase C ^b	M-1	M-6
Percent Carbon Converted to CO ₂	103	111	102	unknown	99.5	99.1	99.1
Carbon dioxide (Theoretical EF ^b)	0.94	0.88	0.65	unknown	1.005	1.11	1.07
INORGANIC COMPOUNDS							
Carbon dioxide (Empirical EF)	0.97	0.42	0.66	0.77	1.0	1.1	1.1
Carbon monoxide	0.91 x 10 ⁻³	0.29 X 10 ⁻³	0.025 x 10 ⁻³	0.49 x 10 ⁻³	0.7 x 10 ⁻³	0.25 x 10 ⁻³	0.095 x 10 ⁻³
Nitrogen oxide	0.14 x 10 ⁻³	3.0 X 10 ⁻³	5.2 x 10 ⁻³	2.8 x 10 ⁻³	2.6 x 10 ⁻³	1.2 x 10 ⁻³	2.4 x 10 ⁻³
Nitrogen dioxide	0.38 x 10 ⁻³	0.61 X 10 ⁻³	2.1 x 10 ⁻³	0.51 x 10 ⁻³	0.15 x 10 ⁻³	0.47 x 10 ⁻³	0.52 x 10 ⁻³
VOLATILE COMPOUNDS							
Methane	67 x 10 ⁻⁶	20 x 10 ⁻⁶	BD ^c	BD	750 x 10 ⁻⁶	8000 x 10 ⁻⁶	46 x 10 ⁻⁶
Total nonmethane hydrocarbons	160 x 10 ⁻⁶	33 x 10 ⁻⁶	1.5 x 10 ⁻⁶	45 x 10 ⁻⁶	560 x 10 ⁻⁶	460 x 10 ⁻⁶	13 x 10 ⁻⁶
Benzene	11 x 10 ⁻⁶	5.7 x 10 ⁻⁶	BD	BD	16 x 10 ⁻⁶	4.8 x 10 ⁻⁶	1.7 x 10 ⁻⁶

^aEmission factor—a dimensionless number that, when multiplied by the weight of explosive or propellant material, detonated or burned, results in the weight of analyte expected.

^bTheoretical EF (emission factor) if all carbon is converted to CO₂.

^cBD - below detection limit.

Table 5 Propellant Burns: Maximum Emission Factors^a for Semivolatile Analytes.

Analyte	BangBox		Phase A	Manufacturing Residue		
	Double Base	Composite	Triple Base	Phase B	Phase C ^b	Phase C
SEMIVOLATILE COMPOUNDS						
2,4-Dinitrotoluene	BD ^c	10×10^{-3}	BD	BD	160×10^{-3}	1.2×10^{-3}
2,6-Dinitrotoluene	14×10^{-3}	3.7×10^{-3}	BD	BD	140×10^{-3}	BD
2,4,6-Trinitrotoluene	50×10^{-3}	BD	BD	BD	64×10^{-3}	BD
2-Nitronaphthalene	54×10^{-3}	13×10^{-3}	BD	3.7×10^{-3}	83×10^{-3}	BD
N-Nitrosodiphenylamine	1500×10^{-3}	35×10^{-3}	BD	19×10^{-3}	27×10^{-3}	0.14×10^{-3}
1,3,5-Trinitrobenzene	NA ^c	NA	BD	NA	53×10^{-3}	BD
2-Nitrodiphenylamine	BD	NA	BD	BD	13×10^{-3}	BD
4-Nitrophenol	0.69×10^{-3}	0.41×10^{-6}	BD	BD	NA	NA
1-Nitropyrene	BD	20×10^{-3}	BD	NA	BD	BD
Naphthalene	BD	1400×10^{-3}	BD	1500×10^{-3}	540×10^{-3}	19×10^{-3}
Benz[a]anthracene	BD	BD	BD	38×10^{-3}	140×10^{-3}	BD
Benzof[a]pyrene	900×10^{-3}	BD	BD	23×10^{-3}	81×10^{-3}	BD
Pyrene	NA	NA	BD	71×10^{-3}	320×10^{-3}	BD
Phenol	4400×10^{-3}	3800×10^{-3}	BD	8000×10^{-3}	— ^d	3.4×10^{-3}
Dibenzofuran	0.26×10^{-6}	0.28×10^{-6}	BD	0.26×10^{-6}	120×10^{-6}	BD
Diphenylamine	BD	BD	BD	20×10^{-3}	310×10^{-3}	0.11×10^{-3}

^aEmission factor—a dimensionless number that, when multiplied by the weight of explosive or propellant material, detonated or burned, results in the weight of analyte expected.

^bBD - below detection limit.

^cNA - not a target analyte.

^d—Phenol was lost in the extraction of the semivolatile.

Table 6 Propellant Burns: Semivolatile Analytes Detected and Maximum Recovery in Fallout Pans (ng/g).

Analyte	Phase A	Manufacturing Residue		Phase C	
	Triple Base	Phase B	Phase C ^a	M-1	M-6
SEMIVOLATILE COMPOUNDS					
2,4-Dinitrotoluene	BD	700	58	900	410
2,6-Dinitrotoluene	BD	BD	7.9	36	BD
2,4,6-Trinitrotoluene	BD	BD	120	0.38	1.0
2-Nitronaphthalene	BD	BD	8.8	0.14	0.18
N-Nitrosodiphenylamine	BD	6.7	BD	BD	20
1,3,5-Trinitrobenzene	BD	BD	18	BD	0.009
2-Nitrodiphenylamine	BD	17	BD	0.29	1.1
4-Nitrophenol	BD	BD	NA ^c	NA	NA
1-Nitropyrene	BD	BD	BD	BD	0.009
Naphthalene	BD	390	34	5.5	9.6
Benz[a]anthracene	BD	BD	94	0.1	2.2
Benzo[a]pyrene	BD	BD	8.4	BD	1.1
Pyrene	BD	510	17	BD	0.36
Phenol	190,000	16	--- ^d	BD	0.15
Dibenzofuran	BD	29	80	BD	53
Diphenylamine	BD	2.7	21	6.9	26
Ethyl centralite	96,000	NA	NA	NA	NA
Nitroglycerin	43,000	310	BD	NA	NA
Nitroguanidine	55,000	BD	NA	NA	NA

^arepresents ng of analyte per g of fallout material.

^bBD - below detection limit.

^cNA - not a target analyte.

^d---Phenol was lost in the extraction of the semivolatile.

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SECTION 1. INTRODUCTION

1.1 Demilitarization Stockpile Situation

1.1.1 Size, Storage, and Treatment

The military services possess a massive munitions demilitarization inventory which has reached 200,000 short tons and grows by 25,000 short tons annually, despite ongoing demilitarization operations. The stockpile's growth is expected to accelerate as an expected drawdown of U.S. forces in Europe begins and stocks in our European depots are retrograded. The ammunition logistics support network is presently experiencing several consequences. First, the storage capacity of depot igloo facilities has reached saturation, prompting the need for outdoor storage. Second, many munitions and propellants deteriorate with age and are subject to spontaneous detonation or ignition, with the attendant safety and environmental risks. As the triservice manager for demilitarization, the U.S. Army continues to cope with this problem, traditionally using open burning (OB) and open detonation (OD) thermal treatment procedures. OB and OD have historically proven to be the fastest, safest, most reliable, and least expensive of any demilitarization procedures within existing technology and are well understood by depot munitions specialists.

1.1.2 Environmental Issues and RCRA Permitting

Within the past several years, OB/OD operations have been faced with increasing restrictions. Part of these requirements include the need to obtain permits under provisions of the Resource Conservation and Recovery Act (RCRA), subpart X. Because of the absence of definitive data concerning explosive and propellant combustion products, especially trace organics, RCRA permits have been granted an interim status in many instances, and OB/OD activities closed in others. Unless permitted under RCRA subpart X prior to 8 November 1992, all OB/OD operating sites are subject to closure, and the armed forces may lose their only operating means of reducing a significant part of the demilitarization inventory. Additionally, ordnance manufacturing and processing facilities need OB/OD capabilities to treat their reactive waste streams. Without OB/OD data to support permit application evaluation, these permits will be in jeopardy.

1.1.3 Alternative Methods for Demilitarization

A number of alternative methods have been proposed for demilitarization operations. Some have proven environmentally unsound, e.g., washout which produces contaminated wastewater; others have a low thruput or are severely limited in the quantities or types of ordnance which can be treated; and some are exceedingly expensive or are not technologically mature. Most alternative methods being considered to replace OB/OD will not be operational for at least 5 to 7 years. Until these alternative methods are fully developed, tested, and permitted, stocks will grow to unmanageable proportions, unless OB/OD thermal treatment methods continue at an accelerated pace. It is estimated that OB/OD thermal treatment methods can safely and economically process a large part of the current inventory without serious impact to the environment. Once proven environmentally acceptable, OB/OD thermal treatment methods can work in concert with emerging alternative technologies, to solve the current and future demilitarization problems.

1.2 Background

1.2.1 Interim Study

In 1986, an interim field test was conducted at Tooele Army Depot (TEAD), Utah. The purpose of that test was to evaluate several new testing, sampling, and analysis procedures. A wide variety of material was detonated or burned, ranging from hand grenades to 227 kg (500-lb) bombs to artillery propellants. While most detonations were conducted on the surface, a limited number of buried detonations were conducted. The combustion products of these events were sampled by collectors for subsequent laboratory analyses or analyzed by real-time instruments mounted aboard a UH1-D helicopter. While some valuable data were collected on criteria gases, the real benefit of this test was the evaluation of equipment and procedures. The test revealed that the helicopter was unsuitable as an aerial sampling platform because of the vibration, engine vulnerability to airborne particulate matter, and inability to catch some fast-moving plumes. The test also demonstrated that existing assay technologies were not sufficiently refined to detect the very low levels of emittants desired by environmental regulators.

1.2.2 Symposium - Technical Steering Committee

1.2.2.1 In 1988, the U.S. Army Armament, Munitions and Chemical Command (AMCCOM) convened a technical symposium at Salt Lake City, Utah. This symposium drew internationally recognized authorities from the military services, U.S. Environmental Protection Agency (EPA), academia, not-for-profit organizations, and private enterprise. The symposium included representatives with expertise in analytical chemistry, sampling, modeling, explosives and propellants, statistical analysis, and quality assurance. The technical challenges of the earlier tests were reviewed, and alternate strategies and technologies for the next phases of the study were discussed (reference 1). A Technical Steering Committee (TSC) was formed from selected symposia participants, including the EPA. The initial product of the TSC was the list of target analytes from propellant, explosive, and pyrotechnic (PEP) combustion that were of foremost environmental interest.

1.2.3 The BangBox Test Series

The BangBox test provided the initial assessment of state-of-the-art technologies recommended by the TSC as candidates for use during field testing. These technologies highlighted supercritical fluid chromatography/mass spectrometry (SFC-MS), the carbon balance method for determining combustion product emission factors, micropolished stainless steel (SS) evacuated canisters and tanks for collecting air samples believed to contain volatile organic compounds, a sophisticated reflux-extraction process used to extract volatile organic compounds from the SS tanks/canisters, a high-volume sampling train to trap semivolatile organic compounds, and a fixed-wing aircraft (FWAC) package of real-time analyzers, samplers, and collectors.

1.2.3.1 Test Facility

1.2.3.1.1 The test facility selected to test the samplers, collectors, and real-time analyzers was an inflatable building located at Kirtland Air Force Base, Albuquerque, New Mexico. The facility is operated by the Sandia National Laboratories (SNL) and is known as the BangBox (BB). The flexible nature of the building permitted enclosed detonations of small quantities of explosives (227 g (0.5 lb)) and burns of small quantities of propellants (454 g (1.0 lb)) without violating

structural integrity and allowed any combustion products to be sampled for an extended period of time. Equipment used in the BB was that proposed by the TSC.

1.2.3.1.2 As a permanent fixed facility, the BB facilitated the accurate characterization of combustion products. Test personnel were able to calculate the BB volume and determine background levels of species targeted for individual subtests. Since its size was determined, it permitted precise comparison of the carbon-balance method to the more traditional cloud volume method in calculating emission factors.

1.2.3.1.3 The building was serviced with water and electricity. This permitted technicians to clean the test chamber and prevent cross-contamination between subtests, operate all collection and analytical equipment, and document events with high-speed motion picture cameras and video recorders.

1.2.3.2 Test Results

1.2.3.2.1 The highly satisfactory results of the test were published in a final report (reference 3). In addition to providing data on emission products, several important conclusions were drawn.

a. Those sampling, collecting, and analyzing systems selected for subsequent use are capable of providing complete and accurate data. The semivolatile organic sampling train could not be used for field testing because the throughput was much too low for the short duration of sampling the cloud.

b. Trace organic compounds can be accurately and consistently identified and quantified by the SFC-MS. This was confirmed by spiked samples submitted by the EPA's Atmospheric Research and Exposure Assessment Laboratory and analyzed by the chromatography laboratory.

c. The carbon-balance method performed better than the cloud volume method for calculating emission factors (EF) using samples of homogeneous and nonhomogeneous chamber air.

SECTION 2 SCOPE OF TEST

2.1 Overall Test Program (See Appendix K)

2.1.1 Purpose

Although the individual tests each had their own specific purpose and objectives, the broad overall program purpose is to supply waste characterization data for OB/OD permit applications under RCRA subpart X.

2.1.2 Objectives

2.1.2.1 Identify and validate sampling and analytical technology, instrumentation, and procedures needed to provide RCRA subpart X data characterization.

2.1.2.2 Identify and quantify emissions and residues produced by OB/OD thermal treatment methods.

2.1.2.3 Provide input for development and validation of an OB/OD dispersion model.

2.1.2.4 Identify specific items that can be treated by OB/OD thermal treatment methods without adverse environmental impact.

2.2 BangBox Test

2.2.1 Purpose

The OB/OD BB test series was designed to develop and verify the OB/OD thermal treatment method test methods and technology.

2.2.2 Objectives

2.2.2.1 Characterize the BB chamber volume, ventilation rate, and combustion product cloud homogeneity level.

2.2.2.2 Develop and improve proposed air sampling equipment and sample analysis procedures to be used in later phases on the FWAC, for sampling product clouds from large-scale follow-on outdoor OB/OD trials.

2.2.2.3 Refine, standardize, and compare supercritical-fluid chromatography (SFC) and gas chromatography (GC) techniques for extracting and analyzing resins, filters, and soils for trace quantities of semivolatile organic OB/OD combustion products and residues, using mass spectrometer (MS) detectors.

2.2.2.4 Verify adequacy of other standard analytical methods to be used for analyses of gases, particulates, volatile organic compounds, metals, and nonmetals.

2.2.2.5 Identify and quantify specific target analytes for TNT, a double-base propellant, and a composite propellant.

2.2.2.6 Assess polychlorinated dibenzodioxins (PCDDs) and dibenzofurans (PCDFs) levels generated from burning the composite propellant containing high concentration of NH_4ClO_4 .

2.2.2.7 Provide information on the morphology, composition, and size distributions of airborne particulate material generated by OB/OD operations in the BB.

2.2.2.8 Examine, using data produced under controlled conditions, the validity of the proposed Carbon Balance method of calculating emission factors; compare the results with those calculated using the more-conventional Cloud Volume times Concentration method.

2.2.2.9 Identify or develop appropriate program-specific QA/QC procedures.

2.2.2.10 Establish procedures for transport and storage of sample specimens.

2.2.3 Test Matrix

Table 2.1 BangBox Test Schedule

Subtest	Date Conducted
Homogeneity and chamber volume	1 Dec 88
Ventilation rate	5 Dec 88
Equipment and procedure selection	7 Dec 88
Single detonation - 1	31 Jan 89
Single detonation - 2	2 Feb 89
Single detonation - 3	6 Feb 89
Extended background sampling	7 Feb 89
Multiple detonation	8 Feb 89
Double-base propellant burn	9 Feb 89
Foam-attenuated detonation	13 Feb 89
Multiple-tank sampling	15 Feb 89
Composite propellant burn	16 Feb 89

2.3 Field Test Phase A

2.3.1 Purpose

Phase A was designed to be an operational readiness inspection (ORI) conducted under conditions expected during further testing, to verify the field suitability of instruments and procedures selected pursuant to the BangBox test.

2.3.2 Objectives

2.3.2.1 Evaluate the performance of the instrumented FWAC as a sampling platform during large-scale field OB/OD tests.

2.3.2.2 Determine if target species can be adequately sampled and measured above background levels.

2.3.2.3 Evaluate the utility of the carbon-balance method in the field testing environment.

2.3.2.4 Evaluate soil sampling, handling, and assay procedures (e.g. SFC-MS) for field OB/OD tests.

2.3.3 Test Matrix

Table 2.2 Field Test Phase A Test Matrix.

Date (mo-day-yr)	Trial Number ^a	OB or OD Time (MDT)	Amount Fuel (kg-lb)	Length Burn (s)	Comment
06-13-89	M30-OB-O-P1	13:23:00	1424-3140	19	No primer used
	M30-OB-O-P2	15:44:40	1597-3520	17	
06-14-89	M30-OB-1-P1	10:07:19	3144-6980	21	1.4 kg (3.0 lb) M3A1 propellant used as primer
	M30-OB-1-P2	10:20:58	3193-7040	20	
06-20-89	TNT-ODS-O-A	14:28:46	921-2030	NA ^b	Bulk 32-kg (70-lb) blocks
	TNT-ODS-O-B	14:55:24			
06-21-89	TNT-ODS-1-V	09:58:52	898-1980		Flake material
	TNT-ODS-1-II	10:12:12			
	TNT-ODS-1-III	10:22:42			
	TNT-ODS-1-IV	10:43:46			
	TNT-ODS-1-I	10:54:18			

^aAbbreviations used within trial number:

Group 1 Fuel used.

M30 - Triple-base propellant.

TNT - 2,4,6-trinitrotoluene.

Group 2 Type of trial.

OB - Open burning.

ODS - Open detonation - surface.

Group 3 Trial number.

O - Operational readiness inspection.

1 - Trial number.

Group 4 Site number.

P1, P2 - Burn site number.

A, B, I, II, etc - Detonation site number.

^bNA - not applicable.

2.4 Field Test Phase B

2.4.1 Purpose

Field Test Phase B was conducted to confirm selections of instruments and procedures made as a result of Phase A, and to determine if there is a relationship between the BB test data and the field test data.

2.4.2 Objectives

2.4.2.1 Sample and analyze the combustion products of large-scale OB/OD operations which were conducted in a manner representing treatment site practices.

2.4.2.2 Sample and analyze the combustion products of large-scale OB/OD operations which were conducted from suspended detonations.

2.4.2.3 Determine if the field test detonation data can be related to the BB test detonation data.

2.4.2.4 Provide the foundation for establishing a database on TNT and selected propellant combustion products.

2.4.3 Test Matrix

Table 2.3 Field Test Phase B Test Matrix.

Date (mo-day-yr)	Trial Number ^a	OB or OD Time (MDT)	Amount Fuel (kg-lb)	Length Burn (s)	Comment ^b
10-16-89	TNT-ODS-O-1	14:44:00	904-1998	NA ^c	1.8 kg (4.0 lb) of TNT used as primer.
10-17-89	TNT-ODS-1-4	12:41:32			
	TNT-ODS-1-6	12:55:36			
	TNT-ODS-1-2	13:13:04			
10-18-89	TNT-ODS-2-5	11:56:00			
	TNT-ODS-2-3	12:13:00			
	TNT-ODS-2-7	12:28:50			
10-19-89	BMR-OB-0-P1	14:03:27	3017-6652	173	ABL casting powder used as primer.
10-23-89	BMR-OB-1-P1	09:26:00	2993-6598	180	Smokeless powder used as primer.
	BMR-OB-1-P2	09:37:00	3000-6614	240	
		TNT-ODA-O-0	11:13:00	907-2000	NA
10-31-89	TNT-ODA-1-3	10:48:58	909-2004		
	TNT-ODA-1-5	11:02:00			
	TNT-ODA-1-1	11:17:00			
	TNT-ODA-2-4	14:55:00			
	TNT-ODA-2-2	15:09:00			
	TNT-ODA-2-6	15:23:00			

*Abbreviation used within trial number:

Group 1 Fuel used.

TNT - 2,4,6-Trinitrotoluene.

BMR - Propellant manufacturing residue.

Group 2 Type of trial.

ODS - Open detonation - surface.

OB - Open burning.

ODA - Open detonation - suspended.

Group 3 Trial number.

O - Operational readiness inspection.

1, 2 - Trial number.

Group 4 Site number.

P1, P2 - Burn site number.

0,1,etc - Detonation site number.

^bPrimer in addition to fuel amount.

^cNA - not applicable.

2.5 Field Test Phase C

2.5.1 Purpose

Field Test Phase C was conducted to supplement the developing database on TNT and selected propellant combustion products, and to include additional explosives and propellants in the test program.

2.5.2 Objectives

2.5.2.1 Conduct additional TNT detonations to facilitate relating BB test results to field test results.

2.5.2.2 Conduct additional TNT test to establish the reproducibility (between test precision) of TNT OD emissions.

2.5.2.3 Sample and analyze the explosive decomposition products of composition B (comp B) explosive.

2.5.2.4 Sample and analyze the explosive decomposition products of explosive D.

2.5.2.5 Sample and analyze the explosive decomposition products of RDX explosive.

2.5.2.6 Sample and analyze the combustion products of M1 and M6 single-base propellants.

2.5.2.7 Sample and analyze the combustion products of propellant manufacturing residue.

2.5.3 Test Matrix

Table 2.4a Field Test Phase C Test Matrix.

Date (mo-day-yr)	Trial Number ^a	OB or OD Time (MDT)	Amount Fuel (kg-lb)	Length Burn (s)	Comment ^b
08-07-90	TNT-ODS-1-C5	11:41:00	900-1984	NA ^c	1.8 kg (4.0 lb) TNT as primer.
08-08-90	EXD-ODS-O-A0	10:05:53	839-1850		9.1 kg (20 lb) of C4 used as primer.
	TNT-ODS-O-SB	11:36:12	680-1500		1.8 kg (4.0 lb) TNT as primer.
08-09-90	TNT-ODA-1-OA	09:14:21	895-1974		
	TNT-ODA-1-OC	09:26:57			
	TNT-ODA-1-OB	09:41:55			
	TNT-ODS-1-C1	12:53:56	900-1984		
	TNT-ODS-1-C3	13:12:53			
TNT-ODS-1-CO	15:38:00				
08-13-90	TNT-ODS-2-C6	11:07:53	895-1974		
	TNT-ODS-2-C4	11:24:10			
	TNT-ODS-2-C2	11:35:18			
08-14-90	BMR-OB-1-P1	09:42:30	2253-4968	66	0.23 kg (0.5 lb) Unique ^d powder as primer.
	BMR-OB-1-P2	09:54:55	2184-4814	63	
	EXD-ODS-1-A6	12:28:30	916-2020	NA	9.1 kg (20 lb) of C4 used as primer.
	EXD-ODS-1-A2	12:41:55			
	EXD-ODS-1-A4	12:54:30			

^aAbbreviations used within trial number:

Group 1 Fuel used.

- TNT - 2,4,6-Trinitrotoluene.
- EXD - Explosive D.
- BMR - Propellant manufacturing residue.

Group 2 Type of trial.

- ODS - Open detonation - surface.
- ODA - Open detonation - suspended.
- OB - Open burning.

Group 3 Trial number.

- O - Operation readiness inspection.
- 1, 2 - Trial number.

Group 4 Site number.

- C5,A0,etc - Detonation site number.
- P1, P2 - Burn site number.

^bPrimer amount in addition to fuel amount.

^cNA - not applicable.

Table 2.4b Field Test Phase C Test Matrix.

Date (mo-day-yr)	Trial Number ^a	OB or OD Time (MDT)	Amount Fuel (kg-lb)	Length Burn (s)	Comment ^b		
08-15-90	BMR-OB-2-P1	08:31:04	2218-4890	67	0.23 kg (0.5 lb) Unique ^c powder + 1.35 kg (3.0 lb) M2 propellant primers/P1 and P2.		
	BMR-OB-2-P2	08:47:57	2218-4890	68			
	EXD-ODS-2-A1	10:52:00	916-2020	NA ^c	9.1 kg (20 lb) C4 as primer.		
	EXD-ODS-2-A5	11:03:35					
	EXD-ODS-2-A3	11:24:28					
08-16-90	RDX-ODS-1-D1	09:17:45	871-1920		1.8 kg (4 lb) TNT primer.		
	RDX-ODS-1-D5	09:32:55	875-1930			2.27 kg (5.0 lb) C4 primer.	
	RDX-ODS-1-D3	09:46:10	880-1940				
	RDX-ODS-2-D6	13:06:35	899-1982				
	RDX-ODS-2-D2	13:20:45					
	RDX-ODS-2-D4	13:42:10					880-1940
	08-27-90	CMB-ODS-1-B1					13:19:20
CMB-ODS-1-B5		13:35:30					
BM6-OB-1-P1		15:17:25	3184-7020	17			
BM6-OB-1-P2		15:26:40		12			
BM6-OB-1-P3		15:38:00		12			
08-28-90	BM6-OB-2-P1	12:04:20		13			
	BM6-OB-2-P2	12:15:20		13			
	BM6-OB-2-P3	12:25:35		13			

Abbreviations used within trial number:

Group 1 Fuel used.

BMR - Propellant manufacturing residue.
 EXD - Explosive D.
 RDX - 1,3,5-trinitrohexahydro-1,3,5-triazine.
 CMB - Composition B.
 BM6 - M6 propellant.

Group 2 Type of trial.

OB - Open burning.
 ODS - Open detonation - surface.

Group 3 Trial number.

1, 2 - Trial number.

Group 4 Site number.

P1, P2 - Burn site number.

A1, A5, etc - Detonation site number.

^bPrimer amount in addition to fuel amount.^cNA - not applicable.^dND - no data.

Table 2.4c OB/OD Phase C Test Matrix.

Date (mo-day-yr)	Trial Number ^a	OB or OD Time (MDT)	Amount Fuel (kg-lb)	Length Burn (s)	Comment ^b
08-29-90	BM6-OB-3-P1	09:32:00	3184-7020	18	1.35 kg (3.0 lb) M1 propellant as primer.
	BM6-OB-3-P2	09:44:00		17	
	BM6-OB-3-P3	09:58:00		21	
08-30-90	BM6-OB-4-P1	10:32:30	3320-7320	14	1.35 kg (3.0 lb) M1 propellant as primer.
	BM6-OB-4-P2	10:48:10		12	
	BM6-OB-4-P3	11:01:20		12	
09-05-90	BM1-OB-1-P2	11:38:15	3159-6965	17	0.23 kg (0.5 lb) of Unique ^c powder as primer.
	BM1-OB-1-P1	11:52:25		16	
	BM1-OB-1-P3	12:03:50		16	
09-06-90	BM1-OB-2-P1	12:14:00		19	
	BM1-OB-2-P2	12:28:01		17	
	BM1-OB-2-P3	12:40:00		16	
09-18-90	CMB-ODS-1-B0	10:46:05	907-2000	NA ^d	2.27 kg (5.0 lb) C4 as primer.
	CMB-ODS-1-B3	11:04:00	916-2020		
	CMB-ODS-1-D0	11:18:30	907-2000		
	CMB-ODS-2-B6	15:17:50			
	CMB-ODS-2-B2	15:31:05			
	CMB-ODS-2-B4	15:46:20			

^aAbbreviations used within trial number:

Group 1 Fuel used.

BM6 - M6 propellant.

BM1 - M1 propellant.

CMB - Composition B.

Group 2 Type of trial.

OB - Open burning.

ODS - Open detonation - surface.

Group 3 Trial number.

1,2,3,4 - Trial number.

Group 4 Site number.

P1,P2,P3 - Burn site number.

B0,B3,etc - Detonation site number.

^bPrimer amount in addition to fuel amount.

^cNA - not applicable.

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SECTION 3. SPECIFICATIONS

3.1 Description of Facilities/Site

3.1.1 BangBox

The BB consists of two major segments: a test chamber and an airlock (Fig. 3.1). The test chamber is a 16-meter diameter hemisphere constructed of plastic-coated nylon fabric, which is supported on a concrete pad by blower-injected air. The chamber volume is maintained at approximately 927 m³ by adjusting a damper through which air is provided by the blower. The airlock is constructed of wood and is connected directly to the chamber. Passage to the chamber is through a power-operated garage door, which is closed during testing. Airlock doors to the outside atmosphere are airtight, so that chamber pressure can be maintained when the airlock access door is open. Both the airlock and the chamber have electric service, and the chamber has water connections. Figures 3.2 and 3.3 schematically show test chamber and airlock instrumentation, respectively.

3.1.2 DPG Test Grids

DPG was selected for the test location as a result of its available manpower experience in OB/OD operations, the availability of Michael Army Air Field (MAAF) as a staging area for instrumented aircraft, and the availability of munitions at nearby TEAD. DPG is located in the Great Basin, 129 km (80 mi) southwest of Salt Lake City at an altitude of about 1325 m (4347 ft) above mean sea level. The terrain is similar to that encountered in much of the Great Basin region of the western United States, with large expanses of relatively flat terrain interrupted by occasional rugged mountainous regions. The only conspicuous terrain feature in the immediate vicinity of the test grid (Fig. 3.4) is a mountainous area to the northwest, known as Granite Peak.

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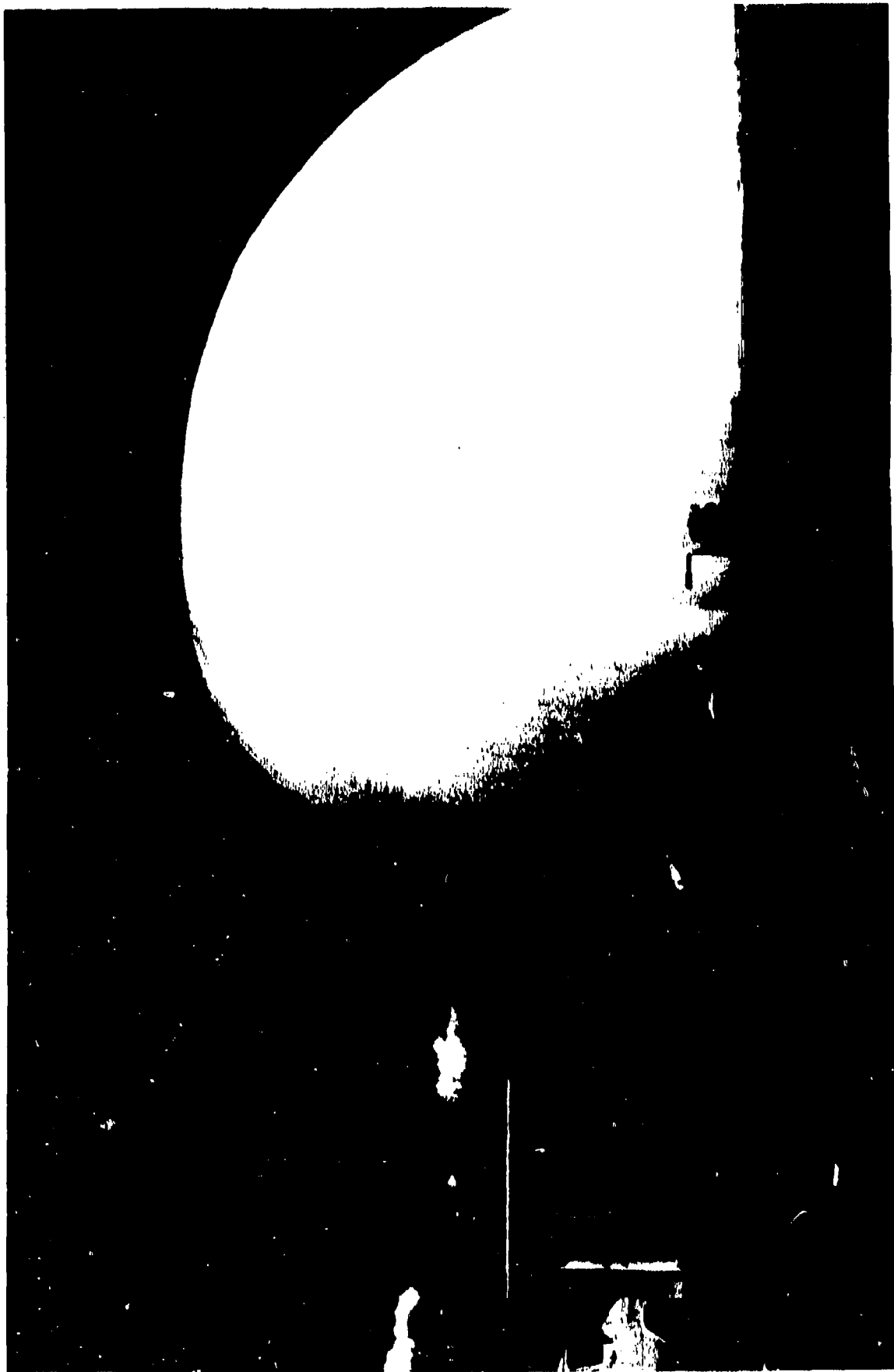


Figure 3.1 SNL BangBox Test Facility Containing Sampling and Real-Time Analysis Equipment.

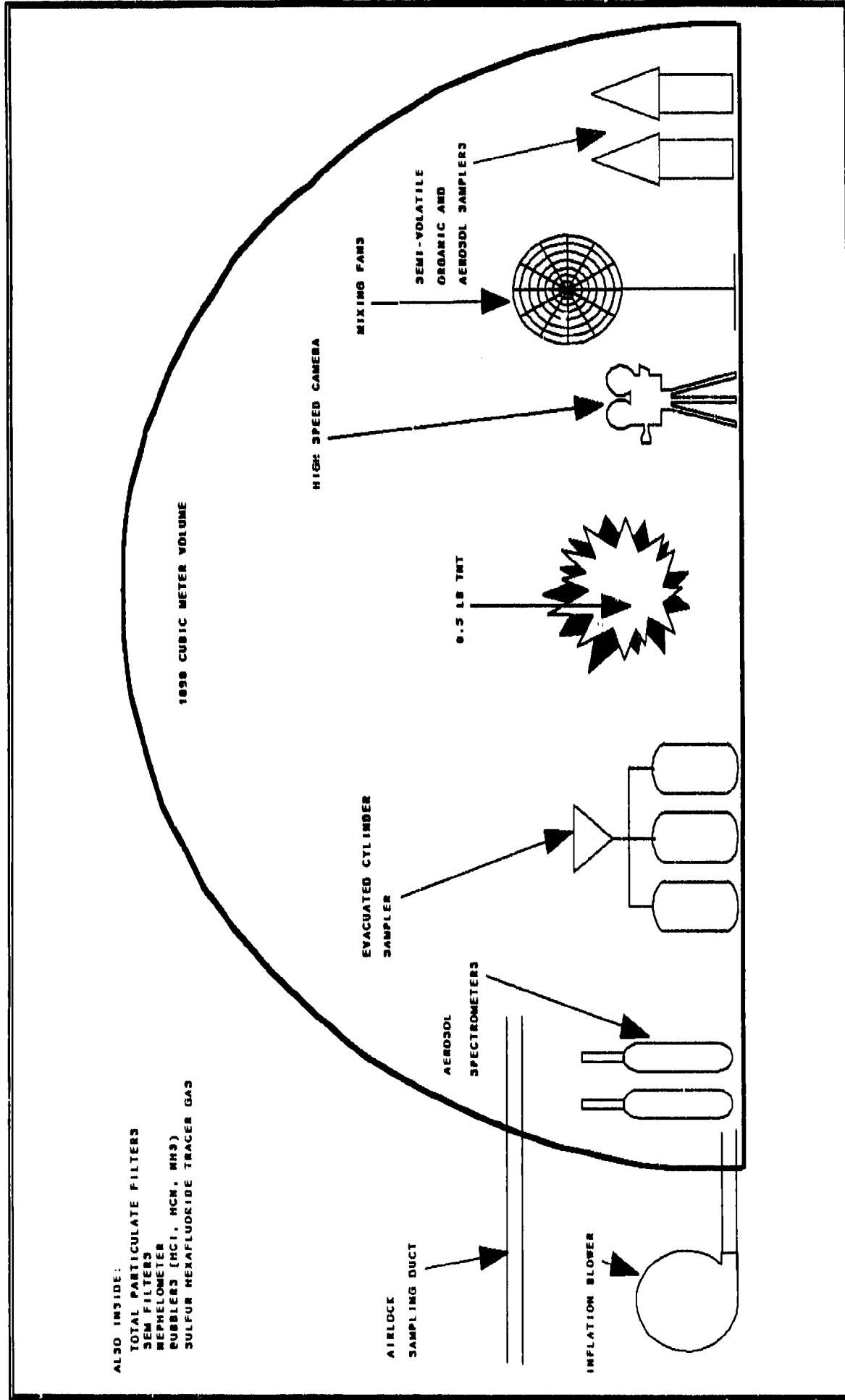


Figure 3.2 SNL BangBox Interior OB/OD Sampling Instrumentation and Equipment.

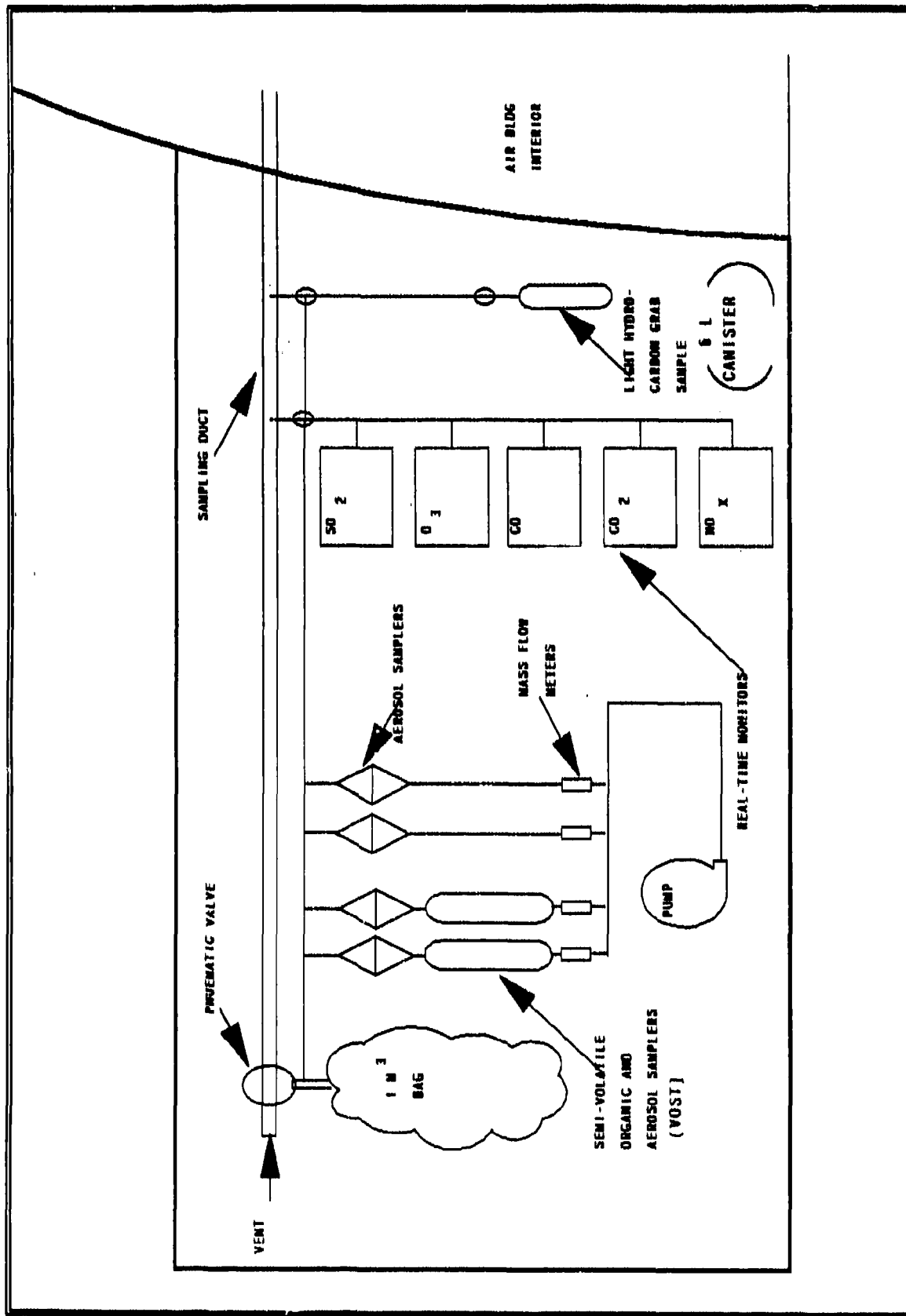


Figure 3.3 BangBox Airlock Instrumentation and Sampling Equipment.

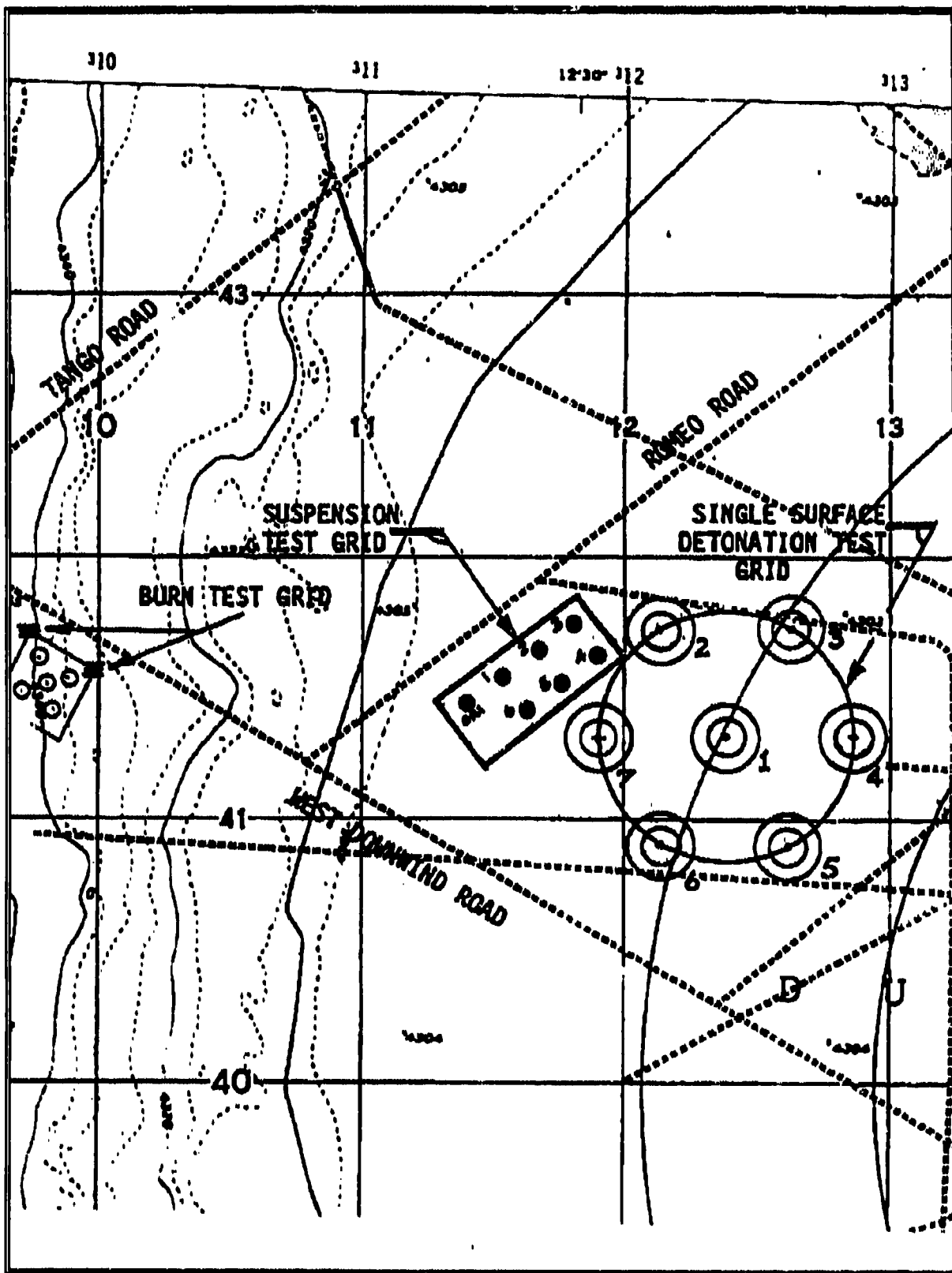


Figure 3.4 OB/OD Test Grid Location.

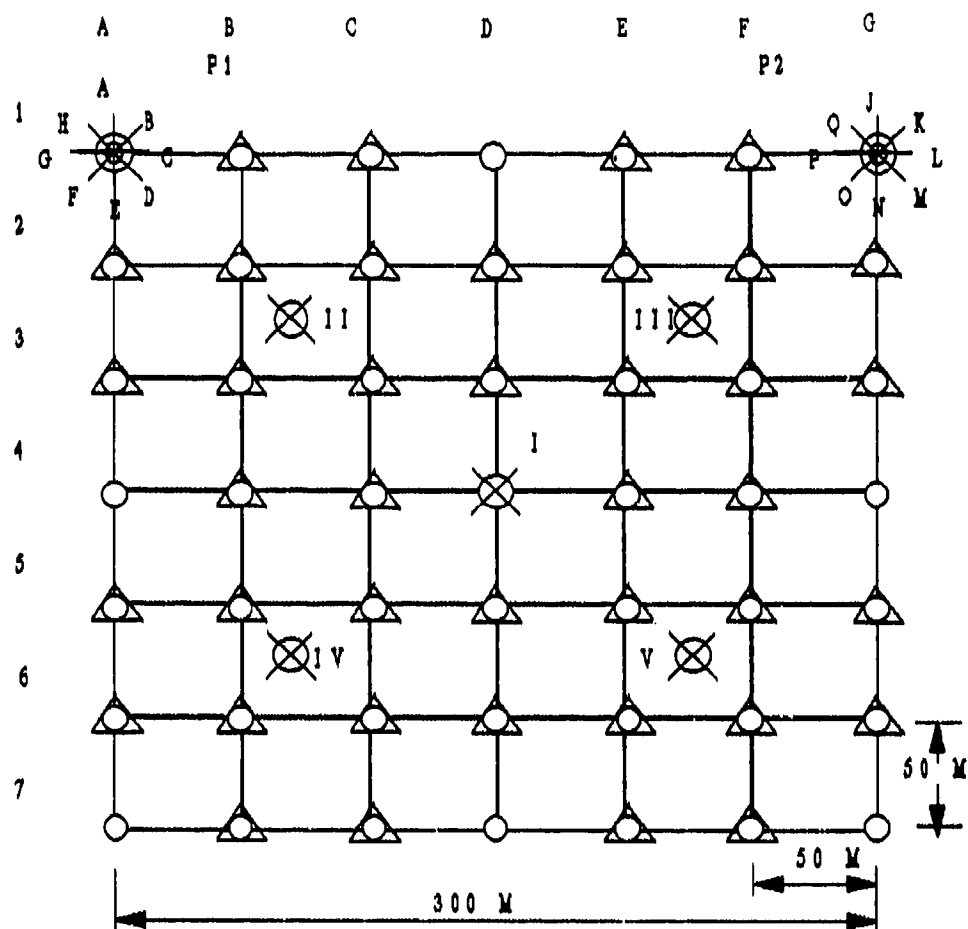
3.1.2.1 Field Test Phase A

The test grid for the triple-base propellant burn was located in an area southwest of the intersections of Tango Road and Romeo Road with West Downwind Road. The TNT detonations were located east of the intersection of Romeo Road and West Downwind Road. This is approximately 15 km (9 mi) from MAAF. The grid was 300 m² (3228 ft²) with sampler positions for TNT located at coordinate points located 50 m (164 ft) apart. Surface soil was sampled at each fallout sampler pan location (Fig. 3.5). The detonation points and burn sites are shown in Figure 3.4.

3.1.2.2 Field Test Phase B

The test grid, with areas designated for the surface detonations, suspended detonations, and propellant burns is shown in Figure 3.4.

3.1.2.2.1 The location relationship of the seven single TNT surface detonation sites is shown in Figure 3.6. Two pretest core samples were taken within 1 m (3.3 ft) of each other to a depth of 2.1 m (7 ft) at the center of each of the seven detonation sites. The layout of the 1 m² (10.8 ft²) fallout pan samples at each of these sites is shown in Figure 3.7. The sampling on the 150 and 200 m (492 and 656 ft) sampling rings was deleted after the ORI test, because quantities of fallout material too small to be useful were collected at these distances during the ORI. However, sampling on the 150- and 200-meter rings was reinstituted in phase C because the concentrations of pollutants in the more distant rings were higher, even though the quantities of fallout were smaller than for the rings at 50 and 100 meters.



LEGEND




-  Detonation Sites
-  Burn Sites
-  Sample Pan Location

Figure 3.5 OB/OD Phase A Soil and Fallout Sampling Location.

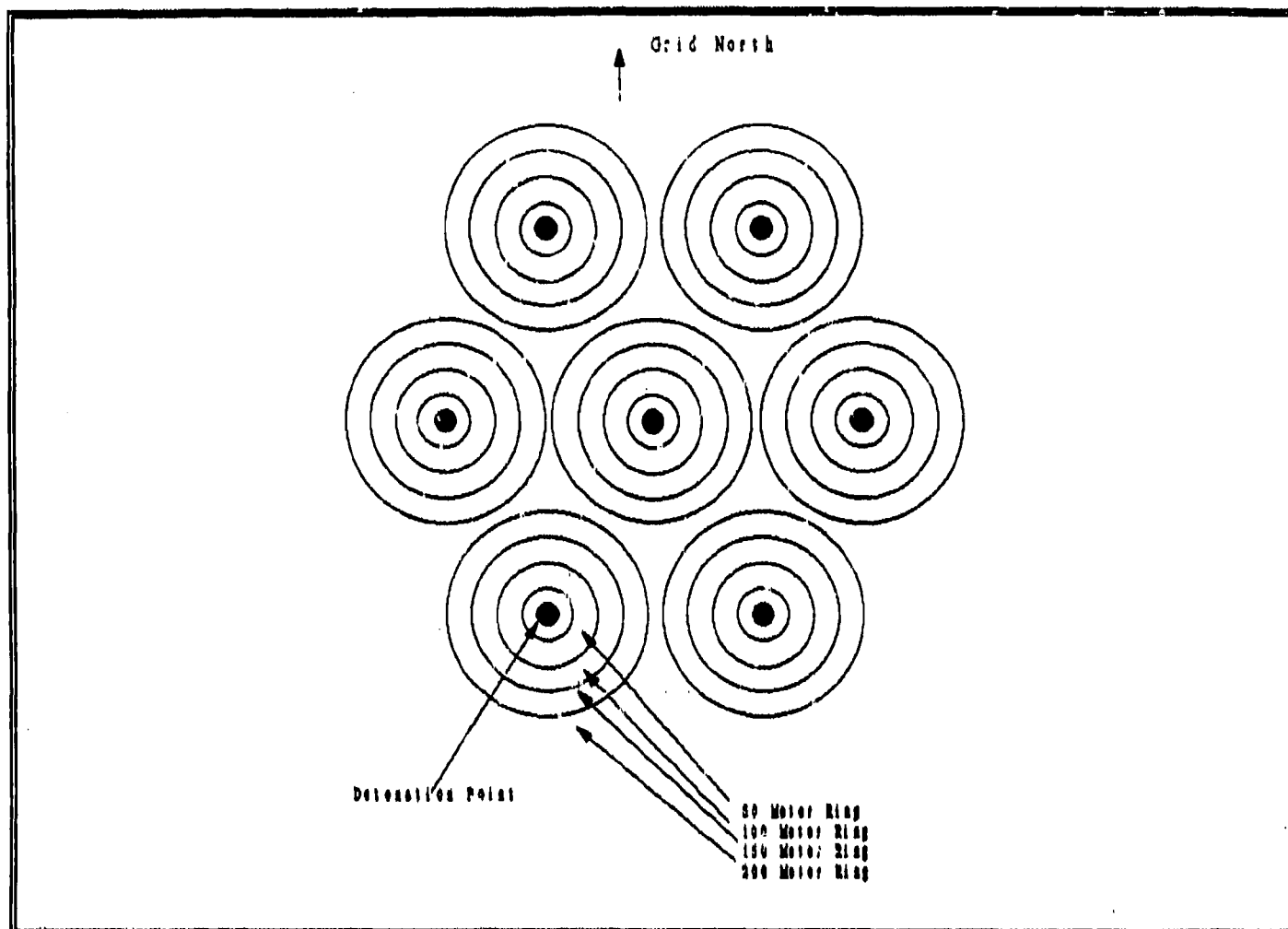


Figure 3.6 OB/OD Phase B Surface TNT Detonation Location Relationships.

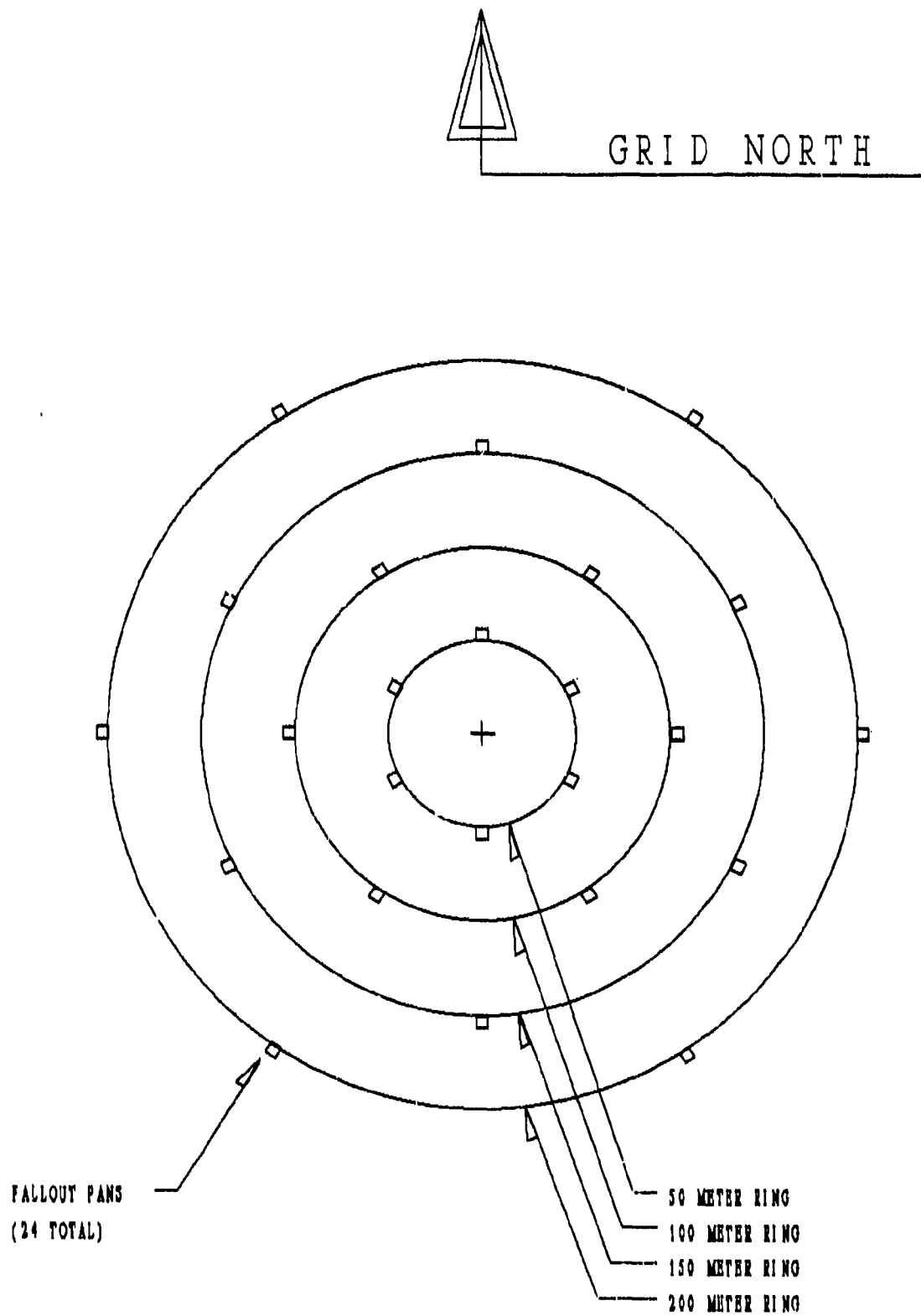


Figure 3.7 OB/OD Phase B Surface TNT Detonations Fallout Pan Layout.

3.1.2.2.2 Posttest samples of the crater and ejecta were taken as follows:

- a. Center of the crater (one sample).
- b. Three meters (9.8 ft) from the center of the crater on four diagonal lines established at 45-degree intervals from grid north (four samples).
- c. One meter (3.3 ft) from the rim of the crater on the diagonal lines (four samples).
- d. Four meters (13.1 ft) from the rim of the crater on the diagonal lines (four samples).

3.1.2.2.3 The sites for the seven single TNT suspended detonations are shown in Figure 3.4. The locations of the pretest and posttest sampling for a typical site are shown in Figure 3.8. This figure also shows the suspension pole locations. The 907 kg (2000 lb) of TNT was suspended approximately 12 meters (40 ft) above the ground, centered between the two poles.

3.1.2.2.4 The locations at a burn site of the 1 m² sputter pans and fallout pan samples are shown in Figure 3.9. Three burn pans were located at each site, each pan 1.2-m (4-ft) wide by 11-m (36-ft) long, and 0.3-m (1-ft) deep. All three pans of propellant at each site were ignited simultaneously.

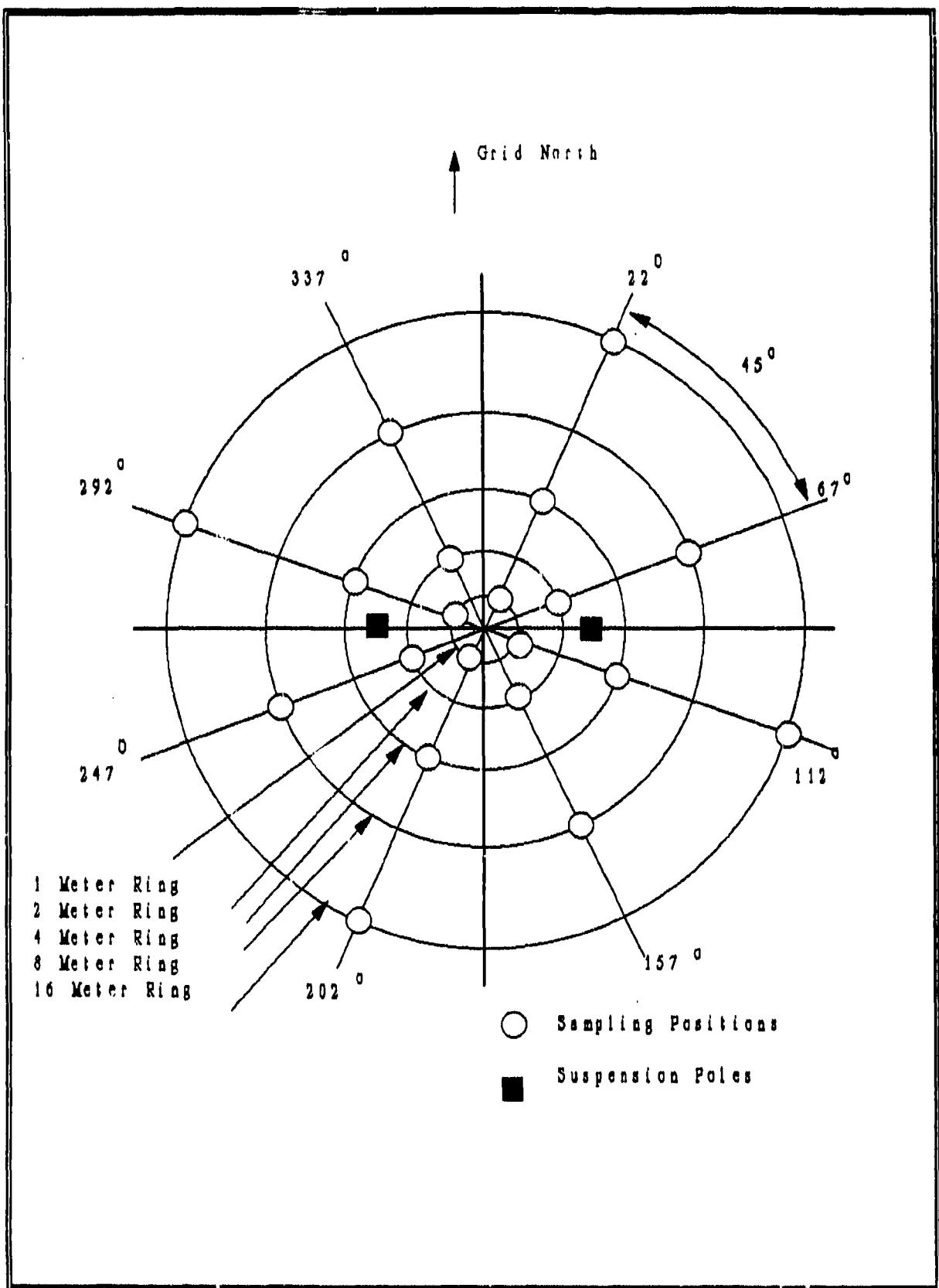


Figure 3.8 OB/OD Phase B Soil Sampling Plan for Suspended TNT Detonations.

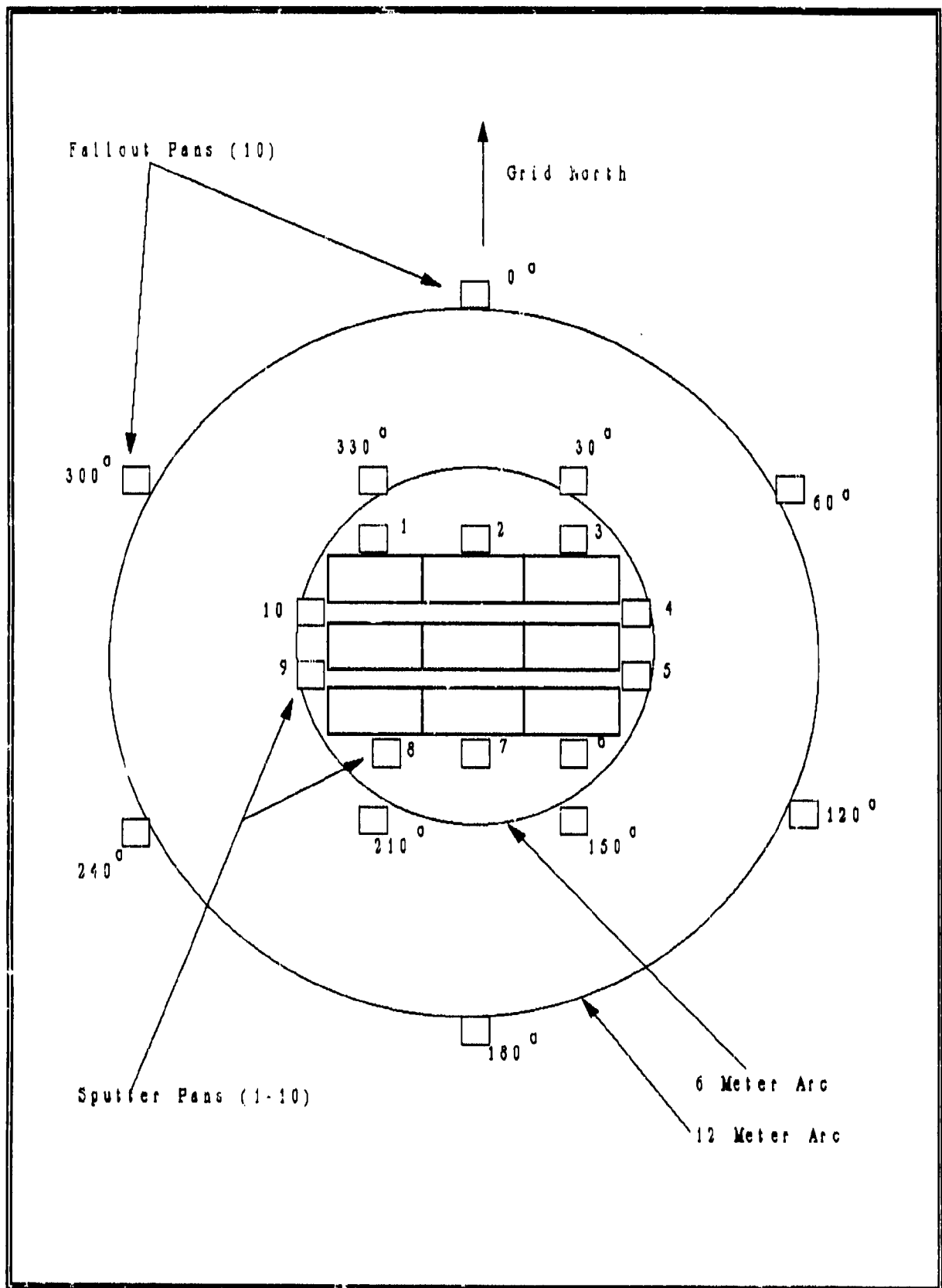


Figure 3.9 OB/OD Propellant Burn Grid Showing Sputter and Fallout Pan Layout.

3.1.2.3 Field Test Phase C.

The test grids for the Phase C trials are shown in Figure 3.10. Surface explosive detonation sites A, B, C, and D were used, respectively, for explosive D, composition B, TNT, and RDX. Only TNT was used at the suspended (aerial) detonation site (Fig 3.10).

3.1.2.3.1 The seven single detonation sites which are in a surface explosive detonation site are shown in Figure 3.11. The fallout pan sampler layout for one of these sites is shown in Figure 3.12.

a. Pretest samples were taken to a depth of 15 cm (6 in), using a 5-cm diameter (2-in) core sampler, as follows:

- (1) Four samples were taken 1 meter (3.3 ft) from grid center at 0, 90, 180, and 270 degrees.
- (2) Four samples were taken 3 meters (9.8 ft) from grid center at 45, 135, 225, and 315 degrees.
- (3) The posttest ejecta sampling of material inside the crater and immediately adjacent to it was taken to a depth where undisturbed soil was encountered.

b. The samples were taken at locations:

- (1) Three meters (9.8 ft) from the lowest visible point of the crater at 0, 90, 180, and 270 degrees from grid north.
- (2) One meter (3.3 ft) from the rim of the crater at 45, 135, 225, and 315 degrees from grid north.

3.1.2.3.2 The suspended explosive detonations, were in the area shown in Figure 3.10. Three detonations were made, each suspended 12 meters (40 ft) above the ground. No sampling of fallout was planned.

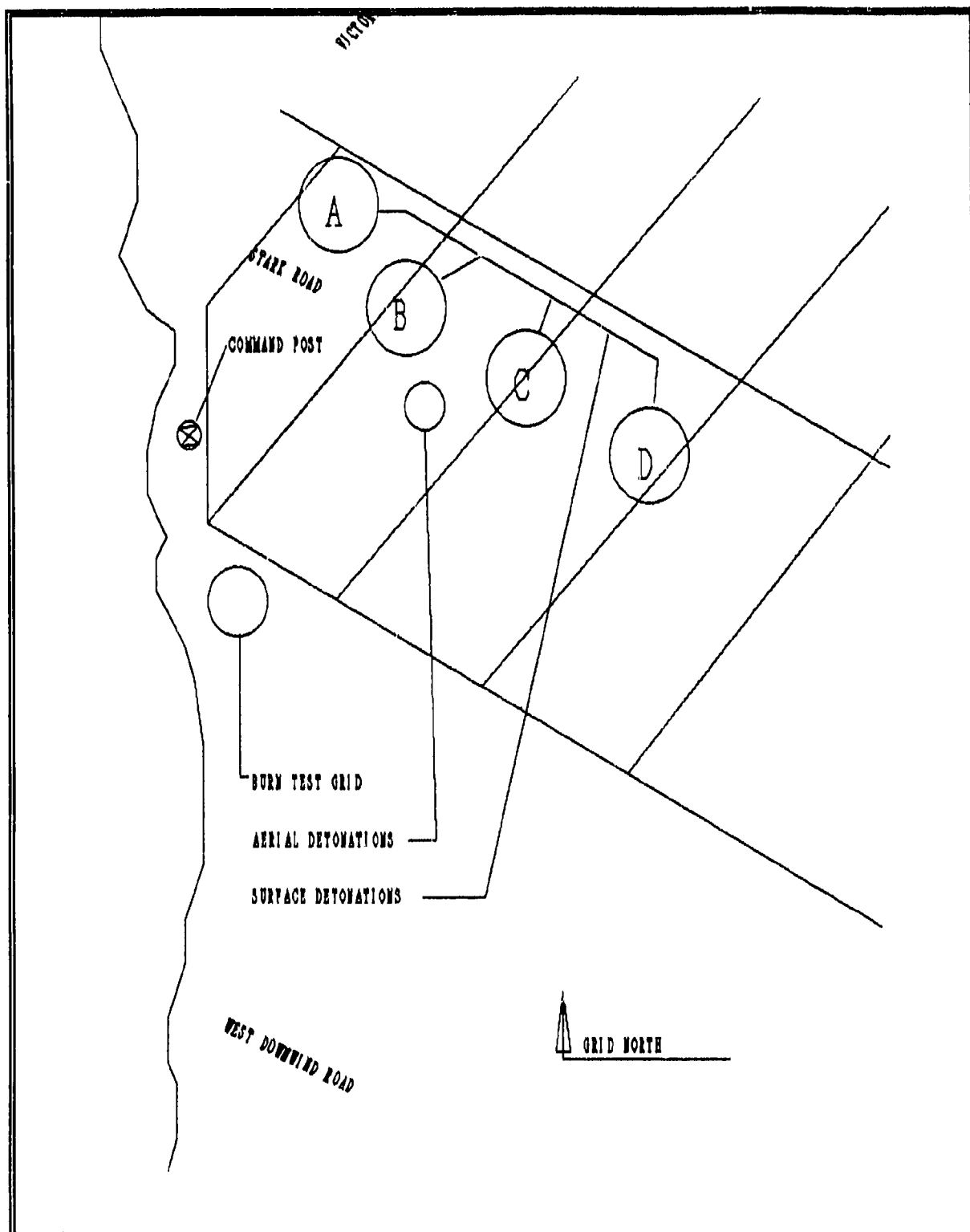


Figure 3.10 Field Test Phase C Locations of Surface Detonations, Suspended Trials, and Propellant Burns.

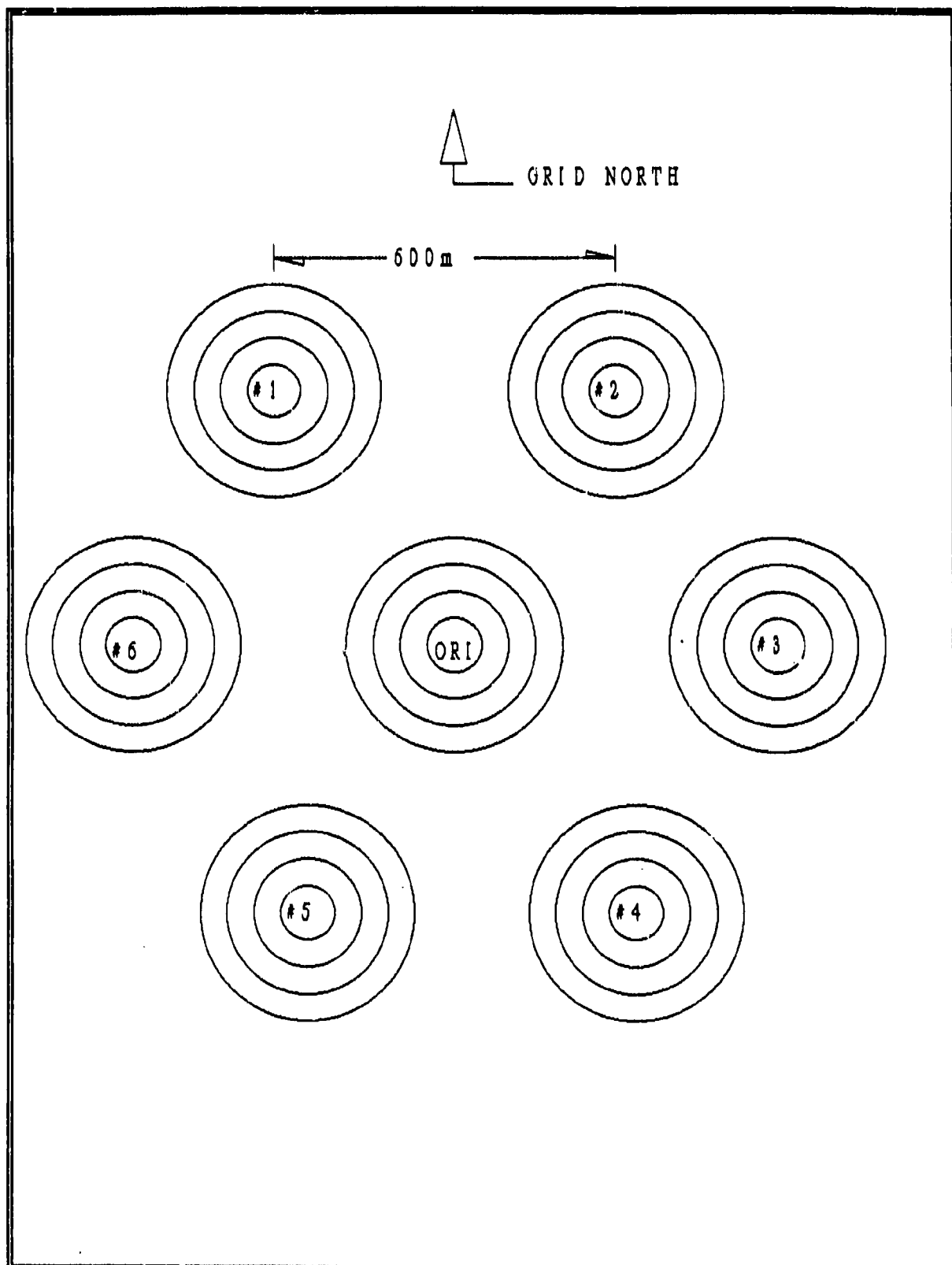


Figure 3.11 Field Test Phase C Relationship of the Seven Surface Detonation Sites Contained in Sites A, B, C, and D of Fig. 3.10.

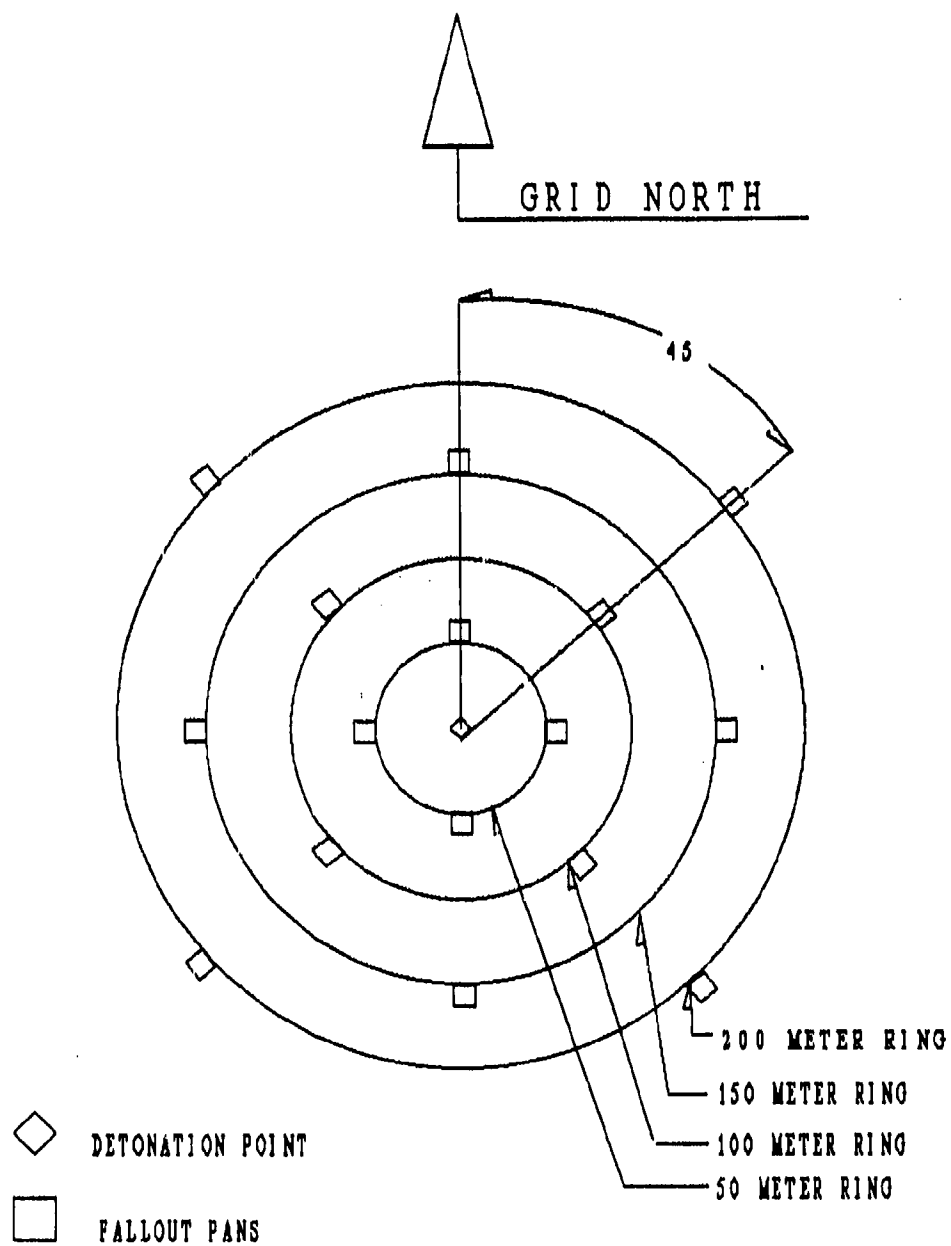


Figure 3.12 Field Test Phase C Fallout Pan Layout for a Detonation.

3.1.2.3.3 The burn test grid area along West Downwind Road had three burn sites, each configured for sampling as shown in Figure 3.9.

3.1.3 Sampling Platform - FWAC

3.1.3.1 Aircraft System Description

The aircraft, instrumented and operated by SNL during this test series, was a Boeing Canada, de Havilland Division, DHC-6 series 300 (Twin Otter) as shown in Fig.3.13. The Twin Otter is a twin-turboprop short take-off and landing, 20-passenger transport aircraft. Maximum take-off weight is 5,670 kg (12,500 lb) and maximum equipment payload, including technical crew, is approximately 1,000 kg (2205 lb). The aircraft has been modified with fastening points to accommodate exterior-mounted instrument packages under both wings and the fuselage. The aircraft is flown with DC-to-AC power inverters onboard, so that conventional instrumentation requiring 115-VAC power can be easily accommodated. Instrumentation is normally carried in up to five standard racks arranged along one side of the aircraft. During the Phase B and C tests, the aircraft was equipped with a "forward-looking" video camera, so that the detonation or burn test and the resulting cloud formation could be recorded during flight. The aircraft accommodates up to five technical-crew members, in addition to a full load of instrumentation and two flight-crew members. A complete description of the various sampling and analysis systems is given below.

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Figure 3.13 SNL Twin Otter Instrumented Fixed-Wing Aircraft for Open-Air OB/OD Sampling and Real-Time Gas Analysis.

3.1.3.2 Aircraft Gas and Aerosol Sampling Probe

The aircraft was equipped with an exterior-mounted inlet sampling probe for collection of both gas and particle samples. The sampling and transport system is shown schematically in Figure 3.14. The probe system was designed to provide a continuous flow of exterior air to the analytical instruments in the aircraft cabin. In addition to supplying the various continuous monitoring instruments, the tube is used to supply input to other sampling systems, such as evacuated canisters, sampling bags, and filter ports. The sampling system consists of five main components: (1) the external probe, (2) the transport tube, (3) the sampling valve, (4) the filter sampling section, and (5) a grab sampling bag. In addition, a transition section joins the probe and transport tube and provides a gradual transition between the different tube diameters of these two components. The sampling probe is an aluminum tube with an 8-cm (3-in) outside diameter and 0.3-mm (1/8-in) walls, that extends outside the aircraft boundary layer at a position forward and above the copilot windshield. A pair of long radius bends are included in the probe section to bring it through the roof of the aircraft and into the passenger cabin, so that particle deposition losses are minimized during air transport through the tube.

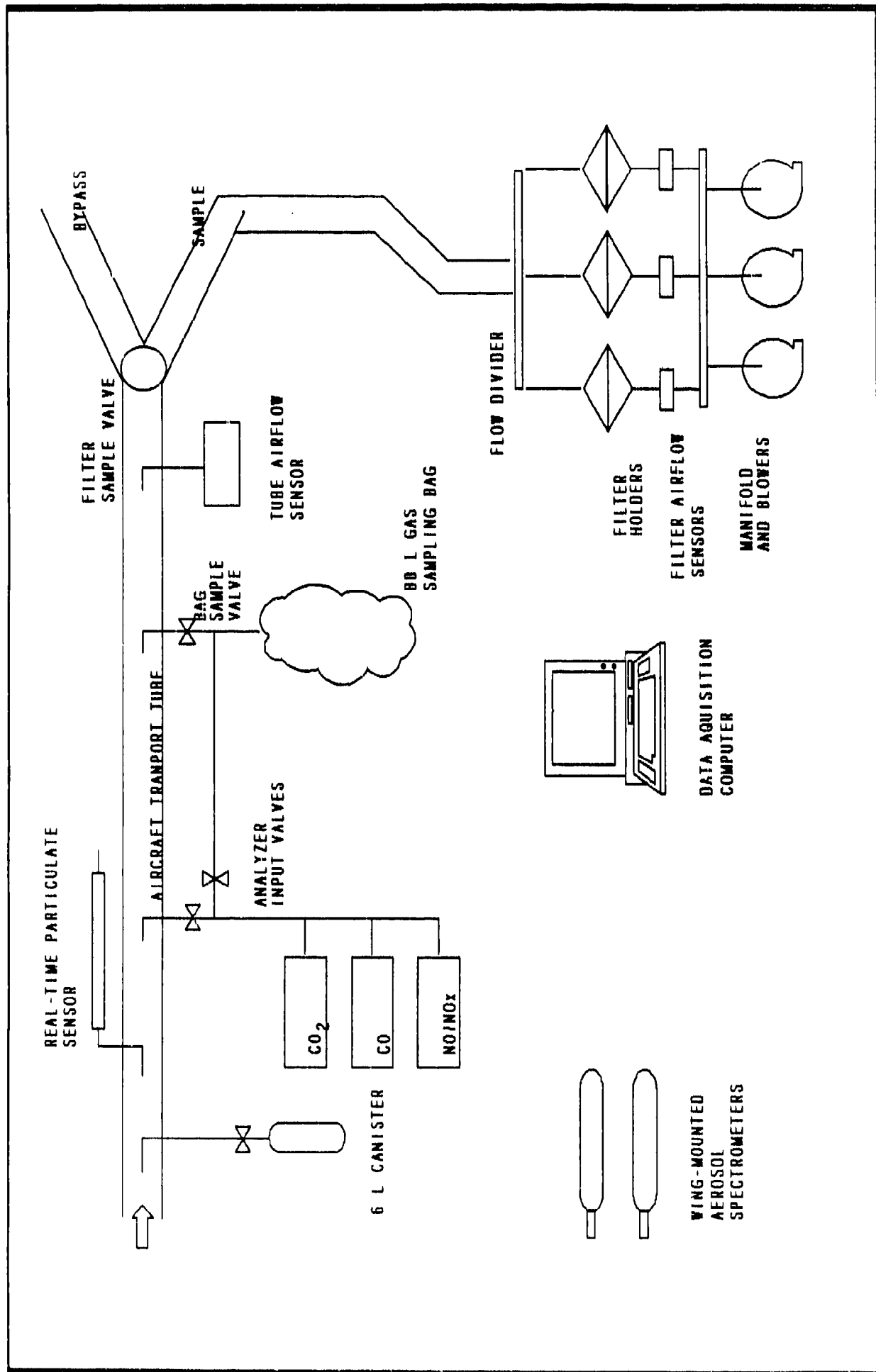


Figure 3.14 Schematic Diagram of Sampling Aircraft Instrumentation.

3.1.3.3 Aircraft Gas and Aerosol Transport Tube

The transport tube, also aluminum, has a 10-cm (4-in) outside diameter and 0.3-mm (1/8-in) walls. It consists of two end-jointed straight sections, each approximately 1.7-m (5.6-ft) long, a total length of 11.2 feet, that terminate in a long-radius 30-degree bend. The straight sections carry the sample flow through the cabin, and the bend leads through the rear cabin bulkhead into the baggage compartment which contains the sampling valve and filter units. The probe, transition, and transport tube sections and valve are joined with compression clamps (Morris Coupling Co., Erie, PA) that provide an essentially smooth interior wall surface from the probe inlet to the sampling valve. Specially designed connections and small probes provide a versatile method for diverting air flow from the transport tube to the analytical instruments and specialized samplers in the aircraft cabin.

3.1.3.4 Aircraft Aerosol Sampling Valve

The sampling valve is a standard 60-degree sliding gate valve (Salina Vortex Corp., Salina, Kansas) and is designed for use in pneumatic conveying applications. The valve body is aluminum, as is the valve plate which slides between nylon pressure plates. The valve position is controlled by a double-acting pneumatic cylinder with quick dump exhaust valves. Control air for the cylinder is supplied through electrically actuated solenoids. One discharge port of the valve is connected to the filter sampling section and the other discharges directly into the rear compartment. The inlet probe and transport tube is continually flushed through a bypass outlet whenever filter sampling is not in progress.

3.1.3.5 Aircraft Filter Port

The filter sampling section consists of three parts: (1) the flow divider, (2) the filter holders, and (3) the vacuum manifold and blowers. The flow divider is attached directly to one port of the sampling valve. It provides for the symmetrical attachment of three 20 by 25-cm (8 by 10-inch) clamshell-type filter holders. These are standard high-volume sampler filter holders (General Metal Works, Village of Cleves, Ohio), except that the inlets have been modified to allow them to be easily connected to and disconnected from the flow divider. The filter holders are constructed of

electro-polished stainless steel and are used with closed-cell urethane foam gaskets and special retaining straps to prevent the closure system from vibrating loose in flight. A vacuum manifold provides uniform suction for the three filters. The manifold is equipped with a bypass inlet, consisting of a pneumatically-actuated ball valve with an inside diameter of 1 cm (0.5 in.) The actuator for this valve is connected in parallel with that for the sampling valve, but with the opposite sense. Thus, when the sampling valve is closed (bypass position), the manifold bypass valve is in the open position. This prevents overloading the blower motors when not sampling, and when sampling is abruptly stopped, it prevents system backflow that could possibly rupture the filters. Air suction is generated by three 0.56 kW (3/4-HP) straight radial blade electric blowers attached to the manifold. (These blowers were manufactured by Gelman Instrument Company, Ann Arbor, Michigan, but they are no longer available from this manufacturer.)

3.1.3.6 Transport Tube Flow Measurement Instrumentation

The total flow through the transport tube was monitored using a Pitot tube mounted well downstream from most of the specialized instrument sampling connections and aligned on the centerline of the transport tube. The differential pressure was monitored on a magnehelic needle gauge (Dwyer Instruments, Inc., Michigan City, Indiana) and was continuously measured with a pressure transducer (Validyne Engineering Corp., Northridge, California) that provided a voltage signal for the analog data collection system. Voltage output from this sensor was proportional to air velocity through the transport tube. The electronic pressure transducer for the Pitot tube was subjected to periodic calibration checks against an inclined manometer pressure standard. A complete description of the calculations made to determine volumetric flow through the transport tube during filter sampling is given in Appendix A.

3.1.3.7 Probe and Transport Tube Sampling Efficiency

Accurate measurement of the concentration and composition of airborne particles from filter samples requires that aerosol properties not be distorted within the sampling system. This requirement offers particular design challenges for any sampling system that is intended to extract particles from a moving airstream. To minimize the distortion of particle size and mass distributions, the air velocity into the probe inlet must be the same as the relative velocity difference

between aircraft and the air being sampled. This is the "isokinetic" sampling condition. A second consideration is the potential loss of particles at the inlet and in the transport tube between the inlet and the collecting filters. Particle losses to the walls of the tube may arise from sedimentation, static attraction, inertial effects, and diffusion. The dominant mechanism of particle loss depends on particle size, tube flow conditions, and tube size.

3.1.3.8 Particle Sampling Losses

A number of experimental and mathematical studies have been completed on particle sampling losses in tubes. Although they provide some insight into the effects in the sampling system used in this work, the conditions in the published studies are not directly comparable to those in the SNL system. The turbulence intensity published in these studies, as indicated by Reynolds number, is typically less than one-quarter of the level encountered in the aircraft tube sampling system under normal flight speeds. Particle transmission efficiency through the probe inlet and tube are calculated from selected parameters from several of these studies and are given in Appendix A. Two cases are considered: one for the case of isokinetic entry into the probe and a second for an entry velocity that is 70 percent of the isokinetic rate. An approximate 70-percent isokinetic sampling rate was measured for the Phase A and B tests that were carried out with quartz filter media. A 100-percent isokinetic sampling rate was measured during the Phase C tests, during which Teflon™-coated glass fiber filters were used. The correction for nonisokinetic conditions is taken from the work of Durham and Lundgren (Reference 3). Deposition losses in the probe and transport tube were estimated as a function of particle size from the work of Liu and Agarwal (Reference 4). Tube flow conditions in the referenced report were not the same as during the AMCCOM tests, but the model has other attractive features. One of these is the inclusion of terms that allow for enhanced penetration of very large particles, rather than assuming that losses increase monotonically with increasing particle size. Details of the calculations are included in Appendix A. The sampling and transport efficiency of particles smaller than 1 μm is unaffected by operating conditions. The increased efficiency for particles larger than 1 μm in the 70-percent isokinetic case results from large-particle oversampling. This oversampling is the result of probe inlet velocity conditions and the lower losses during particle transport down the tube under less turbulent conditions. If the increased sampling efficiencies that result from large-particle reentrainment is disregarded, 70-percent isokinetic sampling conditions result in an approximate 50-percent cut point

for the inlet probe and transport tube at about $5\text{ }\mu\text{m}$ in aerodynamic particle diameter. In other words, an estimated 50 percent of the $5\text{ }\mu\text{m}$ aerodynamic diameter particles that enter the tube are transported to the filter. The other half are deposited on the walls of the transport tube and are not resuspended. Many of the larger ($>10\mu\text{m}$) particles that enter the tube are eventually transported down the tube by saltation processes whereby the particles are continually deposited and reentrained down the tube.

3.1.3.9 Aircraft Gas Sampling Bag

A pillow-shaped $125\text{-}\mu\text{m}$ (5-mil) thickness Teflon™ bag (BGI Inc., Waltham, MA) with an approximate capacity of 80-L was positioned upstream from the filters as schematically shown in Figure 3.14. The bag was connected directly into the transport tube through a ball valve and was used to collect a gas sample from the transport tube at the same time an aerosol sample was being collected by the filter system. Gas analyzer input could be selected either directly from the tube or from the bag by a pneumatically controlled three-way valve. This arrangement allowed gas measurements from the bag to be completed in flight immediately after sampling.

3.1.3.10 Real-Time Particle Concentration/Size Measurements

Three instruments were flown on the aircraft to measure aerosol concentrations in real-time. For the Phase A tests, a flash-lamp-type integrating nephelometer (MRI, Model 1550) was connected directly into the transport tube to allow a real-time measurement of aerosol concentration in flight, as schematically shown in Figure 3.14. A flash rate of 8 Hz with an electronics time constant of 10 Hz was used during all cloud penetrations to insure acceptable instrument response. The output of this instrument was continuously recorded with the data acquisition system. For the Phase B tests, a second forward-scattering nephelometer (MIE Instruments, Model RAM-1) was also used in tandem with the integrating nephelometer as a cloud marker. Only the RAM-1 instrument was used during the Phase C tests.

3.1.3.11 Particle Spectrometers

Two laser-type particle spectrometers were externally mounted on the aircraft in a below-wing configuration. Particles in the 0.15 to 3.0 μm diameter range were measured with an active cavity laser system, using both forward- and back-scattered light collection optics (Particle Measuring Systems, model ASASP-100-X). Particles in the 1- to 47- μm diameter range were measured with a similar instrument that uses an external laser beam and forward-scattering light collection optics to measure both particle size and number counts (Particle Measuring Systems, model FSSP-100-X). The FSSP probe is designed so that it incorporates true *in situ* measurement principles and requires no correction for particle transmission or sampling losses in transport to the particle sensing zone. On the other hand, the ASASP probe is not a true *in situ* instrument. However, since it measures particles less than 3- μm diameter and incorporates a dilution air sheath in the sample route to the measurement chamber, particle transport losses are insignificant. Both probes incorporate extremely fast electronics which enable particle count rates in the range of 10^6 Hz. Data streams from both probes were fed to a digital data acquisition system (Particle Measuring Systems, PDS 400) and then to a portable computer hard disc. Data from each probe were averaged separately over a 5-s interval and recorded continuously during cloud penetrations with the aircraft.

3.1.3.12 Aircraft Data Acquisition Systems

3.1.3.12.1 Phase A

During the Phase A test, two data acquisition systems were used to record in-flight data. One system incorporated a 16-bit (0.01-millivolt resolution) analog-to-digital converter (Hewlett Packard, 3497A) and a computer (Hewlett Packard, 9816) to record all continuous voltage data at a sampling frequency of 2 Hz. A second identical computer was used to record digital data from the wing-mounted aerosol spectrometer probes and a long-range navigation (LORAN) unit. The LORAN receiver indicated aircraft position to an accuracy of about 0.5 km every 5 s.

3.1.3.12.2 Phases B and C

During the Phase B and C tests, all data acquisition was performed using a 386-type 20-MHz personal computer, equipped with Lab Tech Notebook™ data acquisition software that incorporated real-time graphical display during flight. While the aircraft was in ambient air and sampling bag

gas measurements were being taken, the data acquisition rate was at 0.2 Hz. During cloud penetration the data sampling rate was increased to 4 Hz in order to more precisely measure the edges of the clouds. The typical aircraft speed during cloud sampling was 50 m/s. This speed, coupled with the 4-Hz sampling rate, corresponds to a spatial resolution of about 13 meters per data interval.

3.1.3.13 Typical Aircraft Sampling Sequence

3.1.3.13.1 Preflight preparations

On a typical test-day, the aircraft and crew departed its operations base at Provo, Utah, Municipal Airport at approximately 0600. After a 30-min flight, the aircraft landed at MAAF for presampling preparations, which included a thorough cleaning of probe and transport tube interior surfaces, filter holders, and gaskets with isopropanol-soaked cotton swabs. Clean preweighed filters were then installed in the holders and placed in position in the filter sampling manifold. Gas instrument warmup and checkout was also completed during this time interval. While the aircraft was on the ground, the gas instruments were continually operated from auxiliary ground power in order to achieve thermal and electronics stability.

3.1.3.13.2 Background Sampling Flight

After takeoff, the aircraft flew at an altitude of 305 m (1,000 ft) above ground level (AGL) in the vicinity of the test grid and began background sampling. Background aerosol sampling involved sampling of about 150 m³ of background air by continuous operation of the filter sampling system for about 20 min. During this interval, initial zero and span calibrations were also completed on the NO_x, CO, and CO₂ instruments. Gas instrument calibration was followed by a sampling period directly from the transport tube to measure ambient gas concentrations. A 6-L grab sample of background air was also collected into a canister directly from the transport tube at this time. The 80-L bag was flushed with ambient air two times and filled a third time. The gas instruments were then switched to sample from the bag for a period of about 5 min or until instrument readings had stabilized on the bag gas concentrations, whichever occurred first. The aircraft was then flown back to MAAF, during which time a final zero and span calibration was completed with the gas

instruments. Following landing at MAAF, the filter holders were removed and taken inside B-48 (the SNL mobile laboratory) and carefully disassembled. The filters were removed and immediately placed in dry-ice storage. The filter holders were reloaded with clean filters and installed again on the aircraft. The aircraft crew then waited for a ready signal from the ground test director to begin the test sampling flight.

3.1.3.13.3 Test Sampling Flight

a. At the ready signal, the aircraft again departed for the test grid area. On arrival at the test grid, air-to-ground radio communication was established with the test officer. The aircraft then began flying an approximate 4- by 6-km (2.5- by 3.8-mi) racetrack pattern over the test site at its typical sampling speed of 50 m/s (90 knots). During this time initial zero and span checks were completed on the gas instruments. During Phase A and B tests, aircraft position was coordinated with the test officer's countdown, so that the detonation site was approximately 2 km (1.2 mi) directly off the left wing with the aircraft at 305 m (1,000 ft) AGL at detonation time. At detonation time, the aircraft continued flying away from the cloud for about 30 s and then turned 180 degrees to the left, which brought it onto a flight track headed directly at the cloud. Elapsed time from detonation to the first aircraft interception of the cloud was typically in the range of 45 to 60 s. This time lag allowed the buoyant cloud to rise up to the altitude of the aircraft and provided an adequate margin of safety for large debris fallout from the cloud prior to aircraft fly-through. During the Phase C tests, the aircraft was flown at a heading pointing directly at the detonation point and was kept at a minimum distance of 2 km (1.2 mi) at detonation time. This flight path was selected in order to allow a videotape record of the detonation to be made with a nose-mounted "forward-looking" video camera on the aircraft. Prior to the first pass through the cloud, the filter blowers were started with the transport tube flow in the bypass mode. On interception with the cloud, the transport tube flow was diverted through the filters for the duration of the cloud transect. The valve to the 80-L bag was opened at the same time so that the bag was filled with a fraction of the total transport tube flow. A diaphragm valve on an evacuated 6-L canister, installed on a sampling port projecting directly into the transport tube, was manually opened when the aircraft intercepted the cloud on the first sampling pass. The valve was left open, allowing the evacuated cylinder to fill to near atmospheric pressure while the aircraft was in the

cloud, after which it was closed. Typically, the aircraft was in the cloud during this first pass for about 3 to 5 s. As the aircraft exited the cloud, both filter and gas sampling bag valves were switched to the bypass position. The aircraft then was put into a short radius in preparation for another cloud penetration.

b. Second, third, and sometimes fourth penetrations were conducted in precisely the same manner as described for the first, except that no 6-L canister samples were collected. Following the third or fourth pass, the aircraft was flown in level flight in the standard racetrack pattern over the detonation site. At this time, the gas instruments were switched to sample from the bag and a canister sample was also taken from the bag, which now contained cloud gases from all three passes. Sampling was continued from the bag for 5 minutes to adequately measure the bag gas contents. The 80-L bag was then flushed two times with ambient air and completely evacuated in preparation for the next detonation.

c. Continuous recording was carried out with the nephelometer and the two wing-mounted aerosol spectrometers while the multiple cloud penetrations were flown. Range changes were made by instrument operators to optimize instrument sensitivity as the cloud became increasingly dispersed with time

d. In a multiple detonation series, the aircraft returned to the preestablished racetrack pattern over the site, while waiting for the next event. At this time, the 80-L bag was flushed two times with ambient air and completely evacuated in preparation for the next test. Following detonation, an identical sampling sequence was followed as described above for each detonation in the test.

3.1.3.13.4 Posttest Activities

a. For phases A and B, at the completion of sampling from the final detonation cloud, the aircraft was flown back to MAAF. During the return flight, a final zero and span check was completed with the continuous gas analyzers. On landing at MAAF, the filter holders were once again disconnected from the sampling manifold and taken to the equipment trailer. The filters were removed and immediately placed in dry-ice storage. Data files were backed up and sample collection forms completed. Following these activities, the aircraft and crew then departed for the

Provo airport, carrying the ice chest containing the exposed filters with them. Upon landing at Provo, the filters were immediately delivered to Alpine West Laboratories (AWL), where they were placed in cold storage prior to weighing, extraction, and analysis.

- b. For phase C, the filters were weighed and put in the freezer at DPG.

3.1.3.13.5 Propellant Test Sampling Differences

Flight activities for the propellant burns were carried out in an identical manner as described for the detonations, with the exception that a shorter elapsed time between burn initiation and aircraft penetration of the cloud was chosen. Usually, the very buoyant propellant clouds were rapidly dispersed. Typically only two aircraft sampling fly-throughs were completed for each burn.

3.1.4 Soil and Fallout Sampling

The specific sampling points for soil and fallout from the detonations and burns are shown on the grid maps in paragraph 3.1.2 and the following paragraphs. The Technical Steering Committee (TSC) considered the assay of every sample and the compositing of samples. One of these considerations was the high expense of analyzing each individual sample from the test area, of more importance was the TSC's unanimous belief that composite sampling would provide the basis for accurately characterizing ejecta and fallout material, and that compositing would be sufficient in developing the methodology required to identify and quantify emittant products from propellant, explosive, and pyrotechnic (PEP) material.

3.2 Explosive and Propellant Material

3.2.1 TNT

TNT was used in the BB and all three field tests for both surface and suspended detonations. While its physical form varied, either flake or block (the product of washout demilitarization operations), for the field tests, the TNT used in the BB tests was virtually pure trinitrotoluene, as

shown by chemical analysis. No individual detonation exceeded 907 kg (2,000 lb). MIL-T-24BC (Reference 5) contains the military specification for TNT.

3.2.1.1 BangBox

BB testing preceded field testing by several months. Less than 23 kg (50 lb) of TNT were consumed during the entire test series. All was received as 227-grams (0.5-lb) demolition blocks, which had to be stripped of protective cardboard wrappings and metal parts before use. Each trial involved one or more single detonations, each having the block suspended approximately 1 m above the surface by a monofilament nylon cord strung from an aluminum rod bracket assembly. The BB trials were conducted as summarized in Table 2.1.

3.2.1.2 Field Test Phase A

3.2.1.2.1 Description

a. Block. The TNT blocks used during Phase A testing were made from reclaimed TNT which had been cast into 32-kg (70-lb) blocks. Most blocks were packaged in cloth/plastic bags inside a metal container. The bags adhered to the sides of the containers and could not be removed. A lesser amount of TNT blocks came in vapor-barrier bags. These blocks were left in their bags because they were friable and would have spilled on the ground if removed.

b. Flaked. Flaked TNT, also made from reclaimed TNT, was packaged in fiber containers, each holding 60 lb.

3.2.1.2.2 Application

a. Block. The metal boxes containing block TNT were stacked 1.0-m (40-in) deep x 0.7-m (26-in) wide x 1.1-m (44-in) high for detonation. Four 454-g (1-lb) blocks of TNT, used as initiators for the stacked TNT, were each double primed with electric blasting caps and placed on top corners of the stack. The block TNT in vapor-barrier bags was also stacked and initiated by double-primed 454-g (1-lb) TNT blocks.

b. Flaked. The flaked TNT was poured into mild-steel cylindrical buckets, approximately 907 kg (2000 lb) of TNT per bucket. Each bucket was approximately 1.2-m (48-in) high x 1.1-m (45-in) diameter and open at both ends, thus resulting in direct contact between the TNT and the soil. The cylinders were each recessed into the ground approximately 15 cm (6 in) and initiated by one 454-g (1-lb) TNT detonation block double-primed with electric blasting caps and placed on top of the flaked material.

c. All trials were conducted as summarized in Table 2.2.

3.2.1.3 Field Test Phase B

A combination of individual surface, sequential surface, and suspended detonations were conducted, again using reclaimed TNT.

3.2.1.3.1 Description

a. Block. The TNT blocks used during Phase B testing were 32-kg (70-lb) blocks cast from reclaimed TNT. All were wet, varied in strength from being fairly solid to being friable, and had an average 18-percent void space between blocks when placed in the cylinders. Their dark color indicated contamination by munitions components such as asphaltum and gums during the reclamation process. The vapor-barrier bags which could not be removed easily remained on the blocks in some instances.

b. Flaked. The flaked TNT, also the product of reclaimed TNT, was dry when received but, like the block TNT, appeared to have been contaminated during the reclamation process.

3.2.1.3.2 Application

a. Block. The blocks were loaded into cylinders similar to those used during Phase A testing, except that leak-proof bottoms had been added to prevent direct contact of TNT with the soil. Flaked TNT was used to fill voids between blocks. The cylinders were initiated by four 454-g (1-lb) TNT blocks placed inside the cylinder, approximately 20-cm (8-in) from the bottom. The detonating

blocks were wrapped with pentaerythritol tetranitrate (PETN) detonating cord which was run through holes drilled in the sides of the cylinders 15 m (50 ft) to a firing point, where it was initiated by a radio-actuated electric blasting cap. The cylinders were set directly on the ground for surface detonations; for suspended detonations, they were hung approximately 12 m (40 ft) above the ground from a wire cable stretched between two telephone poles.

b. Flaked. The flaked TNT was used to fill voids between blocks in the cylinders. No cylinders were loaded with flaked TNT exclusively.

c. All trials were conducted as summarized in Table 2.3.

3.2.1.4 Field Test Phase C

3.2.1.4.1 Description

Again, TNT used during Phase C was reclaimed explosive which had been reprocessed into flakes and blocks. However, this time the blocks were slightly smaller and weighed 28 kg (62 lb).

3.2.1.4.2 Application

Procedures used in setting up testing events were identical to those used during Phase B, with the exceptions that the cylinder diameter had been reduced to 1.0 m (38 in), and that the cylinders for the ORI was filled with flaked TNT. Plastic sheets were spread on the ground to prevent accidental TNT spills from contaminating the soil. All trials were conducted as summarized in Table 2.4.

3.2.2 Composition B

3.2.2.1 Description

Composition B, manufactured from TNT and RDX, is commonly referred to as "comp B". This explosive was used for six surface detonations during Field Test Phase C. The nominal composition of composition B is given in Table 3.1.

Table 3.1

Ingredient ^a	Weight (%)	Carbon Content (%)
RDX	59.5	16.2
TNT	39.5	37.0
Composition D-2 Wax	1.0	85.2

^aWeights are approximate. RDX and TNT are ± 2.0 and wax is ± 0.03 percent.

Application

Received in flaked form, the composition B was loaded into steel cylinders for test detonations, each cylinder containing a maximum of 916 kg (2020 lb). Each cylinder was 96-cm (38-in) high x 122-cm (48-in) diameter, with a 20-cm (8-in) ring at the top to increase its loading capacity. All trials were conducted as summarized in Table 2.4.

3.2.3 Explosive D

3.2.3.1 Description

Explosive D was used for an ORI and six surface detonations in Field Test Phase C. Commonly referred to as "yellow D" because of its yellow color, explosive D is also known by its chemical name, ammonium picrate. It has a propensity to stain, and can cause toxic reactions, thus mandating personal protection for technicians working with it. Because of its low sensitivity, large initiators were used to ensure complete detonation and avoid spreading undetonated explosive throughout the test site. The nominal composition of explosive D is given in Table 3.2.

Table 3.2 Nominal Composition of Explosive D.

Ingredient	Weight (%)	Carbon Content (%)
Ammonium picrate	99.9	29.3
Sulfates	0.1	
Chloroform insoluble impurities	0.1	
Ash (maximum)	0.1	
Water-insoluble material (maximum)	0.1	

3.2.3.2 Application

Received in granular form, explosive D was loaded into steel cylinders for test detonations, each cylinder containing a maximum of 917 kg (2020 lb). Plastic explosive C4 was used to initiate each cylinder. Plastic sheets were placed on the ground to prevent any spillage from contaminating the soil. Explosive D trials are summarized in Table 2.4.

3.2.4 RDX

3.2.4.1 Description

RDX (hexamethylenetrinitroamine) is not present in ordnance items as a pure explosive. RDX used during Phase C was PBXN-6, a mixture of RDX and Viton A™ (hereafter referred to as RDX). The nominal composition of this explosive is given in table 3.3.

Table 3.3 Nominal Composition of PBXN-6.

Ingredient	Weight (%)	Carbon Content (%)
RDX	95.0	16.2
Viton A™	5.0	28.1

3.2.4.2 Application

Granular RDX was delivered in 60-lb (27-kg) pasteboard boxes. It was loaded into steel cylinders 1.2-meters (48-in) high x 1.0-meters (38-in) diameter. Four 0.6-kg (1.25-lb) blocks of C4 explosive were used to initiate each cylinder. RDX trials are summarized in Table 2.4 on page 2-10.

3.2.5 Single-Base Propellant

3.2.5.1 M1 Propellant - Field Test Phase C

3.2.5.1.1 Description

M1 propellant is a single-base propellant normally used with field artillery, howitzers, and guns. This propellant, consisting almost entirely of nitrocellulose, was received in bulk containers in the form of small multiperforated pellets, each approximately 1 cm long, with a diameter of about 0.4 cm. The nominal composition of the M1 propellant used in phase C is shown in Table 3.4.

Table 3.4 Nominal Composition of M1 Propellant.

Component	Weight Fraction %	Carbon Fraction %
Nitrocellulose (13.15 % N)	85.00	25.7
Dinitrotoluene	10.00	46.2
Dibutylphthalate	5.00	69.0
Diphenylamine (added)	1.00	85.2
Potassium sulfate (added)	1.00	0.0
Volatile solvents	1.26	52.1
Residual water (moisture)	0.60	0.0

3.2.5.1.2 Application

The propellant was spread in the three burn pans to a depth not exceeding 8 cm (3 in) and ignited at both ends of the pans. M1 propellant trials are summarized in Table 2.4 on page 2-11.

3.2.5.2 M6 Propellant - Field Test Phase C

3.2.5.2.1 Description

M6 propellant, as delivered to the test site in 27-kg (60-lb) fiber drums, was a single-base propellant manufactured as a multiperforated grain, 1.7 cm long and 0.8 cm in diameter, consisting almost entirely of nitrocellulose. The nominal composition of this propellant is given in Table 3.5. A carbon fraction of 0.293 was calculated from the mass composition and the molecular formulas of the propellant constituents.

Table 3.5 Nominal Composition of M6 Propellant.

Component	Weight Fraction %	Carbon Fraction %
Nitrocellulose	87.7	25.7
Dinitrotoluene	9.7	46.2
Dibutylphthalate	2.5	69.0
Diphenylamine (added)	0.86	85.2
Potassium sulfate (added)	0.74	0.0
Volatile solvents	1.8	52.1
Residual water	<0.32	0.0

3.2.5.2.2 Application

The propellant was spread in the three burn pans to a depth not exceeding 8 cm (3 in) and ignited at both ends. Propellant ignition was accomplished by black-powder trains, which were ignited by electric squibs. M6 propellant trials are summarized in Table 2.4 on pages 2-10 and 2-11.

3.2.6 Double Base Rocket Propellant

3.2.6.1 BangBox

A single burn trial of 454 grams (1 lb) of NOSIH-AA-2, with 26.6 grams (1 oz) of ethylcellulose added, was conducted in the BB. A description of the propellant is given in Table 3.6. A carbon fraction of 0.266 was calculated from the mass composition and the molecular formulas of the propellant constituents. An additional 5.9 percent by weight of ethylcellulose was added to the mixture, with a carbon fraction of 0.585, to simulate actual field practice in OB of this propellant residue.

Table 3.6 Composition of NOSIH-AA-2 Propellant.

Ingredient	Weight (%)	Carbon Fraction (%)
Nitrocellulose	51.0	27.0
Nitroglycerin	38.6	15.9
Triacetin	2.7	49.5
Di-normal-propyl-adipate	1.6	62.6
2-Nitrodiphenylamine	2.0	67.3
Lead salicylate	1.5	34.9
Lead β resorcyate	0.5	32.8
Monobasic copper salicylate	2.0	49.8
Candelilla wax	0.1	85.2
Ethylcellulose (added)	5.9	58.5

3.2.7 Triple-Base Propellant - Field Test Phase A

3.2.7.1 Description

A triple-base gun propellant, M30, was tested during Phase A. A complete description of the propellant is given in Table 3.7. A carbon fraction of 0.178 was calculated from the mass composition and the molecular formulas of the propellant constituents.

Table 3.7 M30 Triple-Base Gun Propellant* Composition.

Component	Weight Fraction (%)	Carbon Fraction (%)
Nitrocellulose (12.6 % N)	28.0	26.5
Nitroglycerin	22.5	15.9
Nitroguanidine	47.7	11.5
Ethyl Centralite	1.5	76.1
Graphite	0.2	100.0
Total Volatiles	0.1	62.0
Total	100.0	17.8

*Radford Army Ammunition Plant Lot No. RAD-65385.

3.2.7.2 Application

The propellant material was placed in a steel burn pan that measured 1.2 m (4 ft) by 11.0 m (36 ft). Approximately 907 kg (2000 lb) was burned in each of two separate burns for the ORI tests. The full test involved the burning of about 3175 kg (7000 lb) of material in each of two separate burns. M30 propellant testing is summarized in Table 2.2 on page 2-5.

3.2.8 Composite Propellant - BangBox

3.2.8.1 Description

A composite rocket propellant, NOSIH-EC, was tested in the BB test. A complete description of the propellant is given in Table 3.8.

Table 3.8 NOSIH-EC Propellant Composition.

Component	Weight Fraction %	Carbon Fraction %
Hydroxyl-terminated polybutadiene (R45M)	8.015	88.8
2,2-Methylene bis(4-methyl)-6-tert-butyl phenol (AO 2246)	0.200	81.1
Diethyl sebacate (DOS)	4.500	73.2
Phenyl di-isodecyl phosphite	0.200	71.2
5-Ethyl-1,3-diglycidyl-5-methyl hydantoin diepoxide (XU-238)	0.300	56.7
Aluminum oxide	1.000	0
Carbon black	0.100	100.0
Ferric acetylacetonate (FeAA)	0.005	51.0
Ammonium perchlorate	85.000	0
Diethylene triamine (DETA)	0.080	46.6
Isophorone di-isocyanate	0.600	64.4

3.2.9 Manufacturing Residue

3.2.9.1 Field Test Phase B

3.2.9.1.1 Description

A variety of propellant types was used during the Phase B test burns. The purpose of mingling propellant and inhibitor materials was to accurately represent procedures used at manufacturing facilities which thermally treat residue as it is generated. The mixtures are defined in Table 3.9. A complete description of the propellants is given in Tables 3.6, 3.8, and 3.10 to 3.13. Carbon fractions of 0.214, 0.213, and 0.212 were calculated from the mass composition and the molecular formulas of the propellants for the ORI burn and the two burns on trial 1, respectively.

Table 3.9 Manufacturing Residues Burned in Field Test Phase B.

Propellant Type	Weight per Trial ^a (lb)		
	ORI P1	Trial I P1	Trial I P2
NOSIH-EC	1528	1599	1584
NOSIH-AA2	1100	1100	1135
NOSIH-AA6 (chunk)	605	495	495
NOSIH-AA6 (sheet)	2574	2574	2574
"Propellant A"	799	784	760
"Ignition propellant"	10	10	10
Cellulose Acetate Inhibitor	36	36	36
TOTAL	6652	6598	6614

^aTrial dates (all 1990): ORI - 19 Oct; Trial 1.

Table 3.10 NOSIH-AA6 Propellant Composition.

Component	Weight Fraction %	Carbon Fraction %
Nitrocellulose (12.2% N)	24.50	27.0
Nitrocellulose (12.6% N)	24.50	26.5
Nitroglycerin	38.80	15.9
Triacetin	3.25	49.5
Di-normal propyl adipate	2.00	62.6
2-Nitrodiphenylamine	2.00	67.3
LC-12-15	3.30	
Copper salicylate 1.60 %		49.8
Lead β -resorcylate 1.70 %		32.8
Candelilla wax	0.10	85.2
Carbon black	0.05	100.0
Aluminum	1.50	0

Table 3.11 "Propellant A" Composition.

Component	Weight Fraction %	Carbon Fraction %
Nitrocellulose (12.6% N)	49.89	26.5
Nitroglycerine	33.59	15.9
Triacetin	7.62	49.5
2-Nitrodiphenylamine	1.45	67.3
Aluminum	3.79	0
Lead salicylate	1.83	34.9
Lead resorcylate	1.44	32.8
Lead 2-ethyl hexoate	0.39	38.9
Graphite (added glaze)	0.03	100.0

Table 3.12 "Ignition Propellant" Composition.

Component	Weight Fraction %	Carbon Fraction %
Nitrocellulose (12.6% N)	68.44	26.5
Nitroglycerine	16.48	15.9
2-nitrodiphenylamine	1.91	67.3
Aluminum	7.30	0
Lead resorcyate	2.78	32.8
Lead salicylate	2.78	34.9
Carbon black	0.31	100.0
Graphite (added glaze)	0.04	100.0

Table 3.13 Cellulose Acetate Inhibitor Composition.

Component	Weight Fraction (%)	Carbon Fraction (%)
Cellulose acetate	75.0	50.0
Diethyl phthalate	16.7	64.9
Triphenyl phosphate	8.3	66.3

3.2.9.1.2 Application

The burn pans, used in phase A, were cleaned by test personnel prior to setup. The composite propellant, placed in the center of the three-pan array, could not be removed from cardboard shipping containers for the 19 October burn. Double-base propellants were placed in the two outer pans. Propellant manufacturing residue trials are summarized in Table 2.3 on page 2-7.

3.2.9.2 Field Test Phase C

3.2.9.2.1 Description

Manufacturing Residue propellants were used in the Phase-C test burns. They were NOSIH-AA2 and N-5. The propellant was in the form of rolls 10 cm (4 in) wide x 38 cm (15 in) diameter x 0.2 cm (0.08 in) thick, which would have been subjected to extrusion if its manufacturing process had

been continued. The mixtures for Phase C are defined in Table 3.14. The nominal composition of these propellants is given in Tables 3.6 and 3.15.

Table 3.14 Manufacturing Residues Burned in Field Test Phase C.

Propellant Type	Weight per Trial (lb)			
	Trial 1 P1	Trial 1 P2	Trial 2 P1	Trial 2 P2
NOSIH - AA2	1092	1014	1014	1014
N-5	3876	3800	3876	3876
TOTAL	4968	4814	4890	4890

Table 3.15 Composition of N5 Propellant.

Ingredient	Weight %	Carbon Fraction %
Nitrocellulose (12.6 % N)	50.0	26.5
Nitroglycerin	34.9	15.9
Nitrodiphenylamine	1.9	67.3
Diethylphthalate	10.5	64.8
Lead ethylhexoate	1.8	38.9
Lead salicylate	0.8	34.9
Candelilla wax	0.2	85.2

3.2.9.2.2 Application

These propellant rolls were laid in the burn pans and ignited at both ends of the pans with a powder train. Propellant manufacturing residue trials are summarized in Table 2.4 on page 2-9 and 2-10.

3.3 Analyte List - Detection Levels

The analyte list and detection levels for the field test are shown in Table 3.16.

Table 3.16 Analyte List and Limits of Detection for Phases A, B, and C Tests.

Chemical Analyte	Analyte List			Limit of Detection in Acetonitrile ng/mL ^a	Limit of Detection in 400g of DPG Test Site Soils. ^b		
	Phase A	Phase B	Phase C		ppbW	ng/mL	
2,4-Dinitrotoluene	TNT, M30	TNT, MR	TNT, Comp-B, RDX, Exp-D, M6, M1, MR	0.07	1	400	
2,6-Dinitrotoluene				0.05	1	400	
2,4,6-Trinitrotoluene				0.06	1	400	
2-Nitronaphthalene				0.03	1	400	
N-Nitrosodiphenylamine				0.12	10	4000	
1,3,5-Trinitrobenzene				TNT	0.12	10	4000
2-Nitrodiphenylamine				MR	0.10	10	4000
1-Nitropyrene				TNT	1.30	10	4000
Naphthalene				TNT, MR	0.62	50	20000
Benz[a]anthracene					0.73	1	400
Benzo[a]pyrene					2.30	1	400
Pyrene					0.83	1	400
Phenol ^c				TNT, MR	0.23	1000	400000
Dibenzofuran					0.31	1	400
Diphenylamine		0.21	1		400		
4-Nitrophenol		0.30					
Biaryl		1.15					
Phenanthrene		1.20					
1-Methylnaphthalene		0.62					
2-Methylnaphthalene		0.62					
Ethyl centralite ^d	M30						
Nitroglycerin		MR	MR	0.21	10	4000	
Nitroguanidine ^e							
4-Nitrodiphenylamine		MR					
1,3,5-Trinitrophenol			Exp-D	0.35	20	8000	
RDX, Cyclonite ^f			Comp-B, RDX	0.20	1	400	
HMX, Octogen ^g							

^aDetection limit for SFC/MS under chemical ionization/selected ion monitoring (signal/noise = 3).

^bBased on an acetonitrile extraction of 400 g of soil and then evaporation of the extract to a 1 mL sample for assay. Based on signal to noise ratio of 3 with respect to the soil background.

^cAnalyzed with GC/MS on Phase A.

^dChemical name: N,N'-diethyl-N,N'-diphenylurea.

^eAnalysed as its methyl derivative.

^f1,3,5-Trinitrohexahydro-1,3,5-triazine.

^g1,3,5,7-Tetranitrooctahydro-1,3,5,7-tetrazocine.

3.3.1 Discussion of Detection and Quantification Limits.

The following paragraphs pertain to the 3 to 4 orders of magnitude differences between the "limits of detection" of the analytes in acetonitrile solution and the "limits of quantification" of these analytes when extracted from 400 grams of DPG soil samples. This large difference is normal when extracting and analyzing for analytes in soil samples for the following reasons:

a. Matrix effects and stability of composition, particularly during analytical conditions, must always be considered while assessing the level at which analytes may be reliably measured in a field sample if the analytes are associated with relatively large amounts of "foreign" material.

b. When the analytes are associated with relatively large amounts of foreign material, two matrix effects interact. The first is interference from a relatively large "chemical" background (as distinguished from electronic "noise") in the mass spectra resulting from the complex and somewhat variable mixture of natural soil components, such as humic substances. The second is the difficulty of recovering the analytes from the matrix. Soils, especially fine clay soils such as those at DPG, have a large specific surface with high adsorption isotherms. These conditions make the complete recovery of analytes increasingly difficult as the concentration level of the analyte falls. The background and recovery effects combine to reduce the detection and quantification reliability levels of quantification analysis.

3.4 Sampling/Analysis

3.4.1 Volatile Organics

Both direct and indirect whole air grab samples were collected in passivated 6-L evacuated SS canisters during aircraft penetrations of the plume. Direct samples were collected in canisters that were connected to a 6-mm (1/4-in) SS probe that projected directly into the transport tube as schematically shown in Figure 3.14 on page 3-24. On aircraft contact with the plume, the canister valve was manually opened and the canister filled to ambient pressure. During the Phase B and C tests, indirect whole air grab samples were also collected from the Teflon™ bag into which multiple plume samples were composited. Following completion of the plume sampling and a 10-s

purge to clear the line of ambient gas, a gas sample was drawn from the bag through a length of Teflon™ tubing into the evacuated canister. The 6-L canisters were immediately shipped to the Oregon Graduate Institute of Science & Technology for gas transfer and chromatographic analysis for CO, CO₂ and C₁ through C₁₀ hydrocarbons.

3.4.1.1 Measurement of CO₂, CO, and CH₄ was done by a GC-FID-M (FID - Flame Ionization Detector) method using a Carle Instrument Model 211-M. The CO₂ and CO are methanated over a hot nickel catalyst at 400°. The conversion of the CO₂ and CO is 100% to CH₄. However, the absolute calibration is done against National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) standards for each compound. The method is very sensitive, and precision is excellent since the method is used for long-term global monitoring of the ambient atmosphere where high precision is necessary. The precision of analysis is; CH₄ @ 1700 ppbv ±0.2%, CO @ 100 ppbv ±3%, and CO₂ @ 345 ppmv ±0.3%.

3.4.1.2 The C₂ - C₁₀ volatiles were measured by a different GC (using EPA's TO-14 compendium method) with no conversion to methane, but rather direct detection of each of the eluting compounds by flame ionization. A complete list of volatiles is available for every analysis (Appendix E); however, for the sake of brevity, "target" toxic species such as benzene and toluene were selected to show overall trends in volatile emissions from the various test conducted.

3.4.2 Semivolatile Organic Sampling and Analysis

3.4.2.1 Filter Description

Semivolatile organics were collected on the three 20-cm by 25-cm filters positioned at the termination of the aircraft transport tube. A complete description of the transport tube, valve, and flow measurement system is given in section 3.1.3. Quartz-fiber filters (Pallflex Corp, type QAOT) were used during the Phase A and B tests. These filters were pre-fired at 500 °C for at least 1 hour to remove organic material prior to preweighing and sample collection. In order to provide a weight-constant filter medium with which to measure particulate matter loading on the filter, Teflon™-coated glass fiber filters (Pallflex, Type T60A20) were used for sample collection during the phase C tests. Solvent extraction and SFC-MS analysis of blank Teflon™-coated glass fiber filters

showed no appreciable background organic material, so filters were used as received from the supplier and were not solvent-extracted prior to sample collection.

3.4.2.2 Sampling Methods

Almost all explosive tests conducted during field testing included three 907-kg (2000-lb) detonations. The cloud from each detonation was sampled for semivolatile organics during three aircraft passages through the cloud, with an approximate 5-second duration for each pass. The total sampling time in the cloud from all three detonations was about 45 s. To achieve maximum filter loading, the filters were not changed until all three detonation-produced clouds had been sampled. A typical sampling volume for a three-detonation test sequence was usually in the range of 8 to 10 m³ of air for the Teflon™-coated glass fiber filters used in phase C. Sample volumes for the quartz-fiber filters used in the Phase A and B tests were in the range of 6 to 8 m³. The lower sampling volumes for the quartz filters results from the increased airflow resistance through the quartz-fiber filters used during these tests.

3.4.2.3 Postsampling Filter Handling

During the phase A and B tests, the sample filters were removed from the filter holders when the aircraft landed, stored in either aluminum foil pouches or Teflon™ sheets to minimize filter contact with other contaminated surfaces, and placed in dry ice. During the Phase C tests, the filters were removed from the holders and weighed at DPG prior to being placed in dry ice storage. (See section 3.4.4 for additional information on filter weighing procedures.) All filter samples were preserved with dry ice during transport from the field location to AWL.

3.4.3 Real-Time Gases

3.4.3.1 Gas Analyzer Descriptions

Continuous gas analyzers installed on the aircraft and their measurement principle and detection limits are listed in Table 3.17. Gas filter correlation instruments were used for the measurement of CO₂ (Thermo Electron Corporation, model 41H) and CO (Thermo Electron Corporation, model 48). NO_x was measured with a chemiluminescent instrument. For phases A and B, a Columbia Scientific Instruments, model 1600 NO_x analyzer, was used and for Phase C, a Thermo Electron Corporation, model 42 was used. Ozone was measured during the phase B and C tests, using a UV absorption instrument (Thermo Electron Corporation, model 49). The CO and NO_x instruments are both certified as EPA equivalent methods, under 40 CFR 53. In-line cellulose filters were used in the air inlets of the CO and CO₂ instruments. An in-line Teflon™ filter was installed in the inlet of the NO_x instrument. The input plumbing pathway to these instruments is schematically shown in Figure 3.14 on page 3-24. The input flow to the gas instruments was manually selectable by an air-driven ball valve, so that air samples could be drawn directly from the transport tube or from the 80-L bag. Valve position was continuously recorded by the data acquisition system.

Table 3.17 OB/OD Real-Time Continuous Monitors Installed on the Aircraft.

Species	Instrument	Measurement Principle	Detection Level ^a
Carbon Dioxide	TECO Model 41H	Gas Filter Correlation	1.2 ppmv
Carbon Monoxide	TECO Model 48		0.1 ppmv
Ozone	TECO Model 49	UV ^b Absorption	5 ppbv
Oxides of Nitrogen	CSI Model 1600	Chemiluminescence	6 ppbv

^aDetection level defined as two times the standard deviation of the instrument noise.

^bUltraviolet

3.4.3.2 Gas Analyzer Calibration Procedures

Zero and span gas readings of each instrument were taken prior to and following each test measurement. Zero gas for the CO₂ instrument was produced by passing ambient air through a soda lime scrubber. A zero CO gas stream was produced by passing ambient air through a heated catalytic oxidation unit which converted all ambient CO to CO₂. A zero NO_x stream was produced by pumping ambient air through a scrubbing column containing a mixture of silica gel, activated charcoal, and Purafil™. Working-level span gases were also carried on the aircraft so that pretest and posttest zero and span gas checks could be conducted in flight. The CO and CO₂ span gases

were referenced to NIST standard gases in the possession of the Oregon Graduate Institute of Science & Technology. The NO span gas was measured with the NO_x instrument immediately following a multipoint calibration against a certified NO bottle standard. The NO level in the span cylinder measured by the calibrated instrument then became the assigned span value for the duration of the test series.

3.4.3.3 Gas Data Calculations

Multipoint calibrations with certified gas standards were completed on the CO₂, CO, and NO_x instruments prior to the onset of the test period in order to document instrument linearity over their working ranges. Daily instrument response factors were calculated from the pretest and posttest zero and span checks by the following formula,

3.1 Gas Data Calculation.
$$M = \frac{S}{\left(\frac{V_{si} + V_{sf}}{2}\right) - \left(\frac{V_{zi} + V_{zf}}{2}\right)}$$

where:

M = instrument response factor (ppm volt⁻¹)

S = span gas value (ppm)

V_{si} = initial span reading (volt)

V_{sf} = final span reading (volt)

V_{zi} = initial zero reading (volt)

V_{zf} = final zero reading (volt)

Daily instrument response factors were calculated and used in favor of a single-response factor over the duration of the experiment. Past experiences have shown that, although the linearity of the instrument remains constant, daily electronics drift with varying temperature inside the aircraft can yield less accurate measurements when a single response factor is used. The use of a daily response factor that is derived from a daily two-point calibration (zero and span) takes daily instrument drift into account and yields a more accurate measurement of the particular gas. Gas concentrations in the bag were determined by calculating at least a 2-minute average instrument voltage reading while

the instrument was sampling from the 80-L bag. The starting point of the average was after the instrument had stabilized on the bag reading. The average voltage was then multiplied by the instrument response-factor. The same calculation was performed on the ambient air sample collected in the bag during the background flight. The ambient air gas concentration level was then subtracted from the cloud sample level to derive a background corrected cloud concentration level for each particular gas. Complete details of these calculations are given for a representative test case in Appendix C.

3.4.4 Airborne Particulate Matter

3.4.4.1 Gravimetric Analysis

Efforts were made to quantify the amount of particulate matter collected on the filters used for semivolatile organic analysis in each of the test series. Only crude estimates of particulate matter weight gain were available from the filter samples collected during the Phase A and B tests; because of the inherent weight instability of quartz filter media. Quartz fibers are susceptible to ambient moisture pickup and loss and thus are not well suited for gravimetric analysis. Teflon™-coated glass fiber filters were selected during the Phase C study in an effort to provide a more precise estimate of particulate loading because they are far less susceptible to environmental changes in humidity and temperature.

3.4.4.2 Weight Change

Filters were weighed prior to and after sample collection and the resultant weight change used as an estimate of particulate matter loading on the filters. A rigorous filter-weighing quality control program was initiated during Phase C to provide estimates of weight uncertainty during the initial and final weighing procedures. All filters were weighed on a precision microbalance (Mettler, model AE-20) with an approximate weighing precision of 100 μ g. Overall weight uncertainty for the combined difference between an initial and final filter weight was about 1.5 mg.

3.4.4.3 Particulate Carbon Analysis

During the Phase A and B tests, a measure of particulate carbon content of the combustion or detonation clouds was determined by combustion analysis of a section of the quartz filter at Sunset Laboratories. This particulate carbon analysis incorporates a two-step volatilization and combustion process in which particulate carbon is burned, evolved as CO_2 , catalytically reduced to methane, and detected with a flame-ionization detector. Differentiation between organic carbon, elemental carbon (soot), and inorganic or carbonate carbon is possible by using a multistep analysis procedure in which the combustion temperature and the carrier gas mix is varied (Johnson et al. 1981, Reference 6).

3.4.5 Aircraft-Based Video

Video recordings of all phase C test events were made with a forward-looking video camera mounted on the nose of the instrumented aircraft. A high speed, variable focal length lens ($f1.0$ to 2.2 , 16 to 160 mm) was used to record the detonation while the aircraft was on a heading toward the detonation point and during subsequent sampling passes through the cloud. An on-screen elapsed timer was also used to mark the detonation and each passage of the aircraft through the plume. Originals of all VHS format videotapes made during the Phase C tests are archived at SNL. Selected video recordings were also made during the Phase A and B testing; however, many of these were made with a hand-held camera and are of less desirable quality than those made during the Phase C testing.

3.4.6 Meteorology

3.4.6.1 Synoptic weather for the test site was briefed each test day at 0700 hours to the test team prior to traveling to the test site by the Atmospheric Science Laboratory detachment at DPG. The briefing covered the wind speed and direction, cloud cover, and temperature gradient from the surface to the aircraft sampling height. The time window for the acceptable conditions for OB/OD testing was provided. The OB/OD test officer maintained radio contact with the weather detachment from the test control point throughout the field testing to avoid any unacceptable test conditions.

3.4.6.2 Standard meteorological surface observations of wind speed and direction, temperature, humidity, barometric pressures, and cloud cover were taken every 15 minutes at the test site. Tethersondes were also taken into the field to measure wind speed and direction, and temperature from the surface to 2000 meters above the ground.

SECTION 4 DATA COLLECTION, ANALYSIS, AND RESULTS

4.1 General Methods

This section covers the development of innovative methodology for the efficient and effective characterization of emissions from OB/OD, thermal treatment operations (carbon balance and supercritical fluid chromatography-mass spectrometry (SFC-MS)), existing methodology (gas chromatography-mass spectrometry (GC-MS)) and conversion factors for soil and air pollutant concentrations.

4.1.1 Carbon-Balance Method

4.1.1.1 *The emission factor (EF) is defined as the mass release of a particular species per unit mass of original explosive or propellant consumed.* The carbon-balance method of calculating EFs, is based on two premises: (1) the mass of carbon available in the explosive or propellant can be accounted for in the masses of the various carbon-containing product species, and (2) the proportional distribution among carbon-containing products within individual microregions of the cloud remains relatively constant, even though the actual values for individual concentrations may be different within different macroregions of the cloud.

4.1.1.2 Based on these two premises, the total volume of the cloud becomes irrelevant in making EF calculations, and the EF of any individual product, *i*, can be estimated by the equation:

Equation 4.1 Calculation of Emission Factor.

$$EF_i = (f_c) \frac{[D_i]}{[C]}$$

where, f_c = mass fraction of carbon in the fuel;

$[D_i]$ = average concentration of product, *i*, in any specific volume element, *j*, of the cloud; and

$[C]$ = concentration of all forms of carbon in the sample, from volume element, *j*.

For example, the maximum EF value calculated for 2,4-dinitrotoluene from Phase B *surface* detonation samples was 8.4×10^{-6} weight units of 2,4-dinitrotoluene (e.g., kg) per weight unit of TNT detonated (kg). (Values used were $f_s = 0.37$, $[D_0] = 797 \times 10^{-6} \text{mg/m}^3$ of 2,4-dinitrotoluene, $[C_c] = 34.95 \text{mg/m}^3$ of carbon. The product of an EF for a given species and the total amount of material consumed gives the total atmospheric release of the species.

The carbon-balance method has great potential for calculating OB/OD combustion product EFs in large-scale outdoor tests because *total volumes of clouds and total concentrations of products over that whole "volume" need not be known; only "grab samples" need to be taken within the cloud* by aircraft sampling. Since CO_2 is by far the major product of combustion, only the net (background corrected) CO_2 and the target analytes of interest need to be measured above background in order to successfully use the carbon-balance method.

4.1.2 Analytical Methods for Semivolatile Organics

Filters, soils, and the contents of fallout collection pans were analyzed either by supercritical fluid chromatography-mass spectrometry (SFC-MS) or gas chromatography-mass spectrometry (GC-MS) to expedite the work and allow comparison between the two methods. Phase C tests that incorporated the thermally labile RDX and explosive D (picric acid) explosives required the use of SFC-MS.

4.1.2.1 Gas Chromatography-Mass Spectrometry

Microbore capillary gas chromatography interfaced with mass spectrometry at its present mature stage of development is currently the most sensitive and broadly applicable general method for the analysis of volatile and semivolatile organic compounds, and it is presently the accepted standard. It suffers, however, from two major deficiencies: (1) inadequate volatility of some compounds of interest, even after modification by derivitization, and (2) analyte thermal decomposition under the required conditions of operation.

4.1.2.2 Supercritical Fluid Chromatography-Mass Spectrometry

Supercritical fluid chromatography-mass spectrometry is a rapidly emerging alternative to GC-MS. SFC-MS largely overcomes the two major disadvantages of GC-MS mentioned earlier by taking advantage of the additional parameters of solvation of the analytes in the supercritical carrier fluid modulated by variations in the pressure (fluid density), and by the addition of chemical modifiers. Furthermore, SFC closely approaches GC in resolving power. SFC suffers a disadvantage in that the much larger volumes of gas produced by expansion of the carrier fluid at the MS interface are more difficult to handle, but that problem is being rapidly overcome with improved technology.

4.1.3 Soil and Fallout Samples

4.1.3.1 Conversion Factors for Soil and Particulate Samples

Soil samples include the pretest (background), ejecta, and fallout samples from the explosive detonations. The particulate samples include the sputter, fallout, and burn pan residue samples from the propellant burns. Analytical results are expressed as mass of analyte per mass of soil or particulate collected. Some useful conversions are as follows:

$\mu\text{g/g}$ or mg/kg = ppm (one part per million by mass or weight)

ng/g or $\mu\text{g/kg}$ = ppb (one part per billion by mass or weight)

pg/g or ng/kg = ppt (one part per trillion by mass or weight).

4.1.3.2 Statistical Treatment of the Data.

All field-test phases provided several estimates of soil concentration for each analyte and for each sample source (background, ejecta, and 50- and 100-meter fallout soil). All data were examined and descriptive statistics calculated. The variance for each of the analyte/sample sources were more nearly equal with a logarithmic transformation; thus, geometric means were used to express averages. Using the transformed data, the analysis of variance (ANOVA) was performed for each analyte to determine if concentration means from the four sample sources were different. Duncan's multiple-range test was used to determine which concentration means were different. When the

analyte concentration values were below the detection limit, they were used as missing values in the statistical analyses. The calculation of the geometric means from only the values above the detection limits provides a positively biased mean, which, for health effect risks considerations are conservative.

4.1.3.3 Ejecta.

Ejecta soil is the soil displaced at the point of a *surface* detonation and redeposited in the crater, in the berm around the crater, and within a few meters of the crater. The volume of the displaced soil was estimated, using an equation developed in the Tooele Army Depot OB/OD Study. The equation is given in Equation 4.2.

Equation 4.2 Volume of Crater

$$V = \frac{\pi}{24} (3 D^2 L + 4 L^3)$$

where V = volume of crater

 D = crater width

 L = crater depth

4.1.3.4 Observations Applicable to all Detonations

The careful observer will note the anomaly of several of the semivolatile organic analytes occurring at concentration levels higher than background in soil fallout pans (which always contain only a few grams of very fine, dry soil particulates or dust) at radial distances in the 150 to 200 m range. The contamination is apparently greater at distances more remote from the detonation rather than the reverse which would seem more logical (of course in absolute terms the amounts are very small by any standard). Moreover, analytes such as TNT and the DNTs occur in levels above background levels in fallout pans from RDX detonations where they are not explainable at all in terms of direct contamination from the primary explosive itself. A possible explanation of these anomalies may lie in the nature of the surface of the dry desert soil at DPG which consists primarily of a very light, fluffy powder when it is dry, i.e. very fine soil particulate. A natural consequence of its fineness is that the particulate has a high specific surface (surface area per unit mass) which increases inversely

with particle size; consequently its adsorptive capacity for foreign matter likewise increases. This fine powdery particulate is easily disturbed and hence transported readily by winds and blast waves, yet its very fineness precludes rapid settling out, so that the very material most easily suspended and slowest to settle, by virtue of its higher specific surface, may carry relatively higher proportions of adsorbed foreign matter. Even the casual observer will note, that whenever a surface detonation occurred, that a component of the blast wave is propagated parallel to the ground surface stirring up a cloud of dust projecting a few meters up into the atmosphere and extending radially out from the blast center several hundred meters. This cloud is the major source of the fallout pan samples at distances beyond the periphery of significant subsurface soil ejection. Furthermore this material has been subject to cross-contamination from previous operations elsewhere in the vicinity at DPG. The factors indicate that fallout pan samples located on the surface, containing these fine particles are primarily samples of the existing surface contamination at DPG rather than representative samples of the contamination from the detonation. Soil fallout samples are probably a composite of (1) soil particles that are in direct contact with the fireball of detonation products, and (2) soil particles from the desert soil that are transported by the blast wave.

4.1.4 Emission Factors

Emission factors are also expressed as a ratio of the mass (weight) of a particular pollutant released to the mass (weight) of explosive or propellant consumed. Since the EF is a ratio, it is a dimensionless value; i.e., the EF for an analyte multiplied by pounds of explosive yields the total pounds of analyte released.

4.2 Explosives

The explosives chosen for study in these OB/OD tests were selected on the basis of the materials in the current demilitarization inventory. Bulk TNT was included in all phases as a baseline for comparison of reproducibility of results from phase to phase. It was originally selected for study because it is the most oxygen deficient of the explosives and thus most dependent on environmental oxygen for combustion; i.e., it represents a worst case for the potential of incomplete combustion and thus the greatest potential for air and soil contamination with detonation products.

4.2.1 TNT Tests - Phases A, B, and C

4.2.1.1 Airborne Release

4.2.1.1.1 Gases

a. Gaseous species measured during the large-scale *surface* and suspended TNT detonations conducted during Phases A, B, and C included carbon dioxide (CO_2), carbon monoxide (CO), and oxides of nitrogen (NO_x). During the Phase B and C tests, cloud ozone (O_3) concentrations were also measured. Summary EF data for *surface* TNT detonations are given in Table 4.2.1 and those for the suspended TNT tests in Table 4.2.2. For the *surface* TNT tests, the data in Table 4.2.1 are a compilation of 18 total; separate measurements, taken during three test phases. The data in Table 4.2.2 represents a statistical summary of 10 measurements accomplished in Phase B and C. Details of the methods used to calculate the gas EFs are given in detail in Appendix C. The minimum, maximum and average EF are given in the tables for each species measured. These EF's are dimensionless, so the reader can calculate values in the units of choice. For example, Table 4.2.1 shows that an average of 0.0036 kg of NO_x were produced for each kg of TNT detonated in Phase A. To calculate the total release of a particular species, multiply the EF by the original weight of explosive or propellant.

Table 4.2.1 Gas Emission Factors for Surface TNT Detonations.

Gas Species	Emission Factors (g/g)		
	Phase A	Phase B	Phase C
CO ₂ - min	1.19	1.27	1.25
CO ₂ - max	1.28	1.33	1.30
CO ₂ - avg	1.26	1.29	1.28
CO - min	0.037 ^a	0.016	0.036
CO - max	0.10	0.054	0.066
CO - avg	0.061	0.042	0.049
NO - min	0.00020	0.00098	0.00087
NO - max	0.0010	0.0016	0.0017
NO - avg	0.00070	0.0014	0.0014
NO ₂ - min	0.00091	0.00079	0.0011
NO ₂ - max	0.0070	0.0016	0.0017
NO ₂ - avg	0.0036	0.0011	0.0014

^aPhase A CO data are taken from 6-L canister data.

Table 4.2.2 Gas Emission Factors for Suspended TNT Detonations^a.

Gas Species	Emission Factor (g/g)	
	Phase B	Phase C
CO ₂ - min	1.33	1.34
CO ₂ - max	1.36	1.34
CO ₂ - avg	1.35	1.35
CO - min	0.0029	0.0032
CO - max	0.016	0.0078
CO - avg	0.0073	0.0069
NO - min	0.0016	0.0021
NO - max	0.0039	0.0024
NO - avg	0.0025	0.0023
NO ₂ - min	0.0012	0.0011
NO ₂ - max	0.0031	0.0013
NO ₂ - avg	0.0021	0.0012

^aNo suspended TNT detonations were done during the Phase A tests.

b. Carbon dioxide EF for the *surface* TNT detonations ranged from 1.19 to 1.33 for all *surface* tests conducted with an overall average of 1.28. This compares to a theoretical CO₂ EF of 1.36, assuming that all the carbon in the TNT is converted to CO₂. A ratio of the actual to theoretical CO₂ EF gives an estimate of the overall efficiency of the detonation. For all *surface* tests, the average detonation efficiency is 0.94, indicating that all but 6 percent of the carbon in the TNT is converted to CO₂. Most of the remaining carbon is in the CO category, as discussed further below. Notably, the TNT molecule carries enough oxygen within it to oxidize only about 37 percent of the TNT carbon to CO₂. A secondary combustion mechanism is responsible for the high carbon conversion efficiencies observed in the tests. This occurs by way of entrainment of oxygen in ambient air into the detonation fireball, where further combustion of TNT carbon occurs.

c. The average CO₂ EF from all suspended TNT detonations was 1.35. The corresponding ratio of actual to theoretical CO₂ yield is 0.99, which reveals an even higher conversion efficiency of TNT carbon to CO₂ than observed for the *surface* TNT tests. A likely explanation for this observed effect is increased air entrainment into the detonation fireball in the suspended tests as compared to the *surface* tests. In the *surface* tests, the fireball has extensive contact with the adjacent soil, which depresses fireball temperatures, entrains soil, and restricts the incorporation of ambient oxygen into the fireball.

d. For the *surface* TNT tests, CO EFs varied between 0.016 and 0.10, with an overall average of 0.049. Inter-test comparisons of average CO EFs from each test phase are quite good and range from a low of 0.042 (Phase B) to a high of 0.061 (Phase C) with a relative standard deviation (RSD) between the three tests of 16 percent. For the *surface* TNT tests, about 2 to 3 percent of the TNT carbon is converted to CO, with about 94 percent converted to CO₂. The balance of carbon is in the other categories such as VOC and particles, as discussed below.

e. Carbon monoxide EF for the suspended TNT Tests are lower than those observed for the *surface* TNT tests. The overall average CO EF from the Phase B and C suspended tests was 0.007. These observations are consistent with the higher detonation efficiencies noted above for the suspended TNT tests. About 0.3 percent of the TNT carbon is converted to CO, with 99 percent converted to CO₂ for the suspended-detonation configuration.

f. Nitric oxide (NO) EFs for the *surface* TNT detonations reveal that averages for each of the three test phases varied by a factor of approximately two. Nitric oxide ranged from a low of 0.2×10^{-3} in the Phase A test to a high of 1.7×10^{-3} in the Phase C test. The overall NO EF average was 1.2×10^{-3} , or about 0.1 percent. Nitrogen dioxide (NO₂) EF results were in the same range as those encountered for NO, with an overall average of 1.9×10^{-3} . A conservative estimate of an NO₂ EF was determined to be (0.0038), or about 0.4 percent, by assuming that all NO released in the detonation is eventually converted to NO₂ by normal atmospheric processes. All calculations on gas EFs assume 100-percent recovery from the 80-L Teflon® sampling bag in the aircraft.

g. A slightly higher EF for NO was observed in the suspended TNT trials as compared to the *surface* trials. The average EF for NO₂ remained the same for the *surface* and suspended detonations, although the *surface* detonation EFs were associated with a larger variability. The larger variability is expected because the NO and NO₂ formed from the fixation of N₂ and O₂ is dependent upon the temperature of the fireball and the availability of O₂. The quantity of soil entrained varied from detonation to detonation and this would also result in variation in fireball temperature from detonation to detonation. In contrast, very little soil was entrained in the suspended tests and the NO and NO₂ EF were quite constant. For the suspended TNT tests, a conservative estimate of total NO₂ release, assuming that all NO is converted to NO₂, is about 0.6 percent.

h. Although measurements of ozone (O₃) were made of both background and plume air collected in the bag, the results were inconclusive and suggest that O₃ is rapidly lost to the bag surfaces. Average ozone (O₃) recovery from the bag is about 41 percent, based on collection and measurement of ambient (40 ppb) O₃ levels. It is likely that O₃ readily reacts with bag surfaces and cloud constituents such as NO and particles; however, the relative importance of these two reaction sinks cannot be ascertained from this data. Here, it is reasonable to assume that the detonation results in a net loss of ozone, since much of the NO produced will ultimately be converted to NO₂ by a reaction pathway that consumes O₃.

4.2.1.1.2 Particulate Matter

a. Results from the filter gravimetric analyses for all phases of TNT testing are given in Table 4.2.3. Data are reported as average particle mass concentrations per unit volume of air sampled in the cloud for both *surface* and suspended detonations. The reported data normally represent an average of three cloud passes per detonation for multiple detonations. Particle mass concentration in the cloud was measured by the aircraft in multiple passes through the cloud starting at about detonation time plus 1 minute (T_0+1) to T_0+4 minutes. Results for *surface* TNT detonations are highly variable and range from an average of 45 mg/m³ in Phase A to 258 mg/m³ in Phase C. It is likely that the marked differences in cloud particle concentrations between the Phase A, B, and C tests are largely influenced by the degree of soil moisture and compaction at the detonation site. Ground crews noted very different soil conditions during the various testing phases. Those sites with loosely packed soil are much more likely to loft soil during the detonation. The suspended TNT detonations clearly loft less soil debris than the *surface* detonations, as evidenced by average cloud particulate loadings of 11 and 37 mg/m³ for the Phase B and C tests, respectively.

Table 4.2.3 Summary of Total Particulate Mass Concentrations for Surface and Suspended TNT Detonations.

Test	Particulate Mass Concentration (mg/m ³)			No. of Filter Samples
	Minimum	Maximum	Average	
Phase A - surface	24	65	45	2
Phase B - surface	35	85	62	3
Phase C - surface	248	268	258	2
Phase B - Suspended	8	16	11	3
Phase C - Suspended	37	37	37	1

4.2.1.1.3 Volatile Organic Compounds

a. A statistical summary of VOC EFs measured during all *surface* TNT detonations in all testing phases is given in Table 4.2.4. A similar summary for all suspended TNT tests is given in Table 4.2.5. Only representative species including methane, total nonmethane hydrocarbons (TNMHC-- the sum of the C₂ to C₁₀ compounds detected), and benzene were selected to show the general

trends in VOC emissions from TNT tests. A representative example of all VOC species detected with a calculation of VOC species EFs is given in Appendix E.

Table 4.2.4 Volatile Organic Compound Emission Factors for Surface TNT Detonations^a.

Species	Emission Factor (g/g)		
	Phase A	Phase B	Phase C
CH ₄ - min	930 x 10 ⁻⁶	360 x 10 ⁻⁶	610 x 10 ⁻⁶
CH ₄ - max	1600 x 10 ⁻⁶	5200 x 10 ⁻⁶	2200 x 10 ⁻⁶
CH ₄ - avg	1500 x 10 ⁻⁶	1200 x 10 ⁻⁶	1500 x 10 ⁻⁶
Number of observations	5	19	6
TNMHC - min	750 x 10 ⁻⁶	500 x 10 ⁻⁶	BD ^b
TNMHC - max	1600 x 10 ⁻⁶	11000 x 10 ⁻⁶	5000 x 10 ⁻⁶
TNMHC - avg	1400 x 10 ⁻⁶	1900 x 10 ⁻⁶	2100 x 10 ⁻⁶
Number of observations	5	19	11
Benzene - min	58 x 10 ⁻⁶	32 x 10 ⁻⁶	0.27 x 10 ⁻⁶
Benzene - max	120 x 10 ⁻⁶	400 x 10 ⁻⁶	130 x 10 ⁻⁶
Benzene - avg	94 x 10 ⁻⁶	93 x 10 ⁻⁶	100 x 10 ⁻⁶
Number of observations	5	19	11

^aEmission factors are expressed in terms of 10⁻⁶ for ease of comparison, e.g., 930 x 10⁻⁶ is equivalent to 0.00093.

^bBelow detection limit.

b. Average methane EFs for *surface* TNT tests are about 0.0015 in all three phases. Similar results were observed for the TNMHC category, with an average EF of slightly less than 0.002. For these tests, the TNMHC category was primarily composed of light hydrocarbons, such as ethane, propane, acetylene, etc., with little or no contribution from toxic VOC species, such as benzene and toluene. The methane and TNMHC categories reveal information concerning the degree of detonation efficiency in much the same manner as the carbon dioxide EF. High conversion efficiency of the carbon in the parent explosive compound to CO₂ is accompanied by low production rates of methane and TNMHC. Benzene EFs for the *surface* TNT tests are about a factor of 10 lower than EFs for methane and TNMHC. The average benzene EF from all tests is very near 0.0001 in all three phases.

Table 4.2.5 Volatile Organic Compound Emission Factors for Suspended TNT Detonations^a.

Species	Emission Factor (g/g)	
	Phase B	Phase C
CH ₄ - min	BD ^b	610 x 10 ⁻⁶
CH ₄ - max	220 x 10 ⁻⁶	2200 x 10 ⁻⁶
CH ₄ - avg	61 x 10 ⁻⁶	1500 x 10 ⁻⁶
Number of observations	13	6
TNMHC - min	BD	BD
TNMHC - max	4800 x 10 ⁻⁶	5800 x 10 ⁻⁶
TNMHC - avg	210 x 10 ⁻⁶	5000 x 10 ⁻⁶
Number of observations	16	6
Benzene - min	BD	8.8 x 10 ⁻⁶
Benzene - max	11 x 10 ⁻⁶	130 x 10 ⁻⁶
Benzene - avg	3.2 x 10 ⁻⁶	62 x 10 ⁻⁶
Number of observations	13	6

^aEmission factors are expressed in terms of 10⁻⁶ for ease of comparison, e.g., 220 x 10⁻⁶ is equivalent to 0.000220.

^bBelow detection limit.

c. Similar data for the suspended TNT tests reveals generally lower average EFs for all detected VOC compounds. Methane EFs are quite variable, with a near 50-fold difference between the Phase B and C tests. Much larger differences also exist for the TNMHC category between Phase B and C suspended tests. Benzene EFs for the suspended TNT tests, at about 0.000003, are lower than those measured for the *surface* tests by about a factor of 30. Benzene is included here as representative of the potentially toxic VOC categories for bulk explosive detonations.

d. In general, the VOC EFs for suspended TNT tests are lower than for the *surface* TNT tests. This is consistent with the so called "detonation efficiency" determined for these two test configurations as discussed earlier. Interaction of the *surface* detonated TNT fireballs with soil materials very likely serves to reduce the duration of elevated temperatures within the fireball, as well as entrainment of ambient air into the fireball. The net result for the *surface* detonations is reduced conversion of carbon in the explosive to carbon dioxide with higher fractions of carbon monoxide and light hydrocarbon formation by incomplete combustion mechanisms.

4.2.1.1.4 Semivolatile Organics

a. EFs for the semivolatile organic target compounds are given in Table 4.2.6 for the *surface* TNT test and Table 4.2.7 for the suspended TNT test. As a conservative estimate, only the maximum value encountered in each test type is given in the table for each test series. In general, for both surface and suspended detonations, the majority of the compounds on the target analyte list were not detected on the filter samples.

Table 4.2.6 Maximum Semivolatile Organic Emission Factors Measured for Surface TNT Detonations^a.

Species ^b	Emission Factor (g/g)		
	Phase A	Phase B	Phase C
2,4-Dinitrotoluene	150 x 10 ⁻⁹	8400 x 10 ⁻⁹	BD ^c
2,6-Dinitrotoluene	19 x 10 ⁻⁹	7100 x 10 ⁻⁹	BD
2,4,6-Trinitrotoluene	220 x 10 ⁻⁹	150 x 10 ⁻⁹	60 x 10 ⁻⁹
2-Nitronaphthalene	80 x 10 ⁻⁹	270 x 10 ⁻⁹	BD
N-Nitrosodiphenylamine	BD	4.4 x 10 ⁻⁹	BD
1,3,5-Trinitrobenzene	BD	BD	BD
2-Nitrodiphenylamine	BD	N/A ^d	BD
1-Nitropyrene	BD	39 x 10 ⁻⁹	BD
Naphthalene	BD	3700 x 10 ⁻⁹	2600 x 10 ⁻⁹
Benz[a]anthracene	2.2 x 10 ⁻⁹	160 x 10 ⁻⁹	100 x 10 ⁻⁹
Benzo[a]pyrene	BD	240 x 10 ⁻⁹	BD
Pyrene	BD	N/A	220 x 10 ⁻⁹
Phenol	BD	5200 x 10 ⁻⁹	BD
Dibenzofuran	BD	85 x 10 ⁻⁹	180 x 10 ⁻⁹
Diphenylamine	N/A	7.7 x 10 ⁻⁹	170 x 10 ⁻⁹
4-Nitrophenol	BD	N/A	N/A
Biphenyl	BD	N/A	N/A
Phenanthrene	BD	N/A	N/A
1-Methylnaphthalene	BD	N/A	N/A
2-Methylnaphthalene	BD	N/A	N/A

^aEmission factors are expressed in terms of 10⁻⁹ for ease of comparison, e.g., 150 x 10⁻⁹ is equivalent to 0.000000150.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels.

^cBelow detection limit.

^dNot included on analyte list for analysis.

Table 4.2.7 Maximum Semivolatile Organic Emission Factors Measured for Suspended TNT Detonations^a.

Species ^b	Emission Factor (g/g)	
	Phase B	Phase C
2,4-Dinitrotoluene	200 x 10 ⁻⁹	BD ^c
2,6-Dinitrotoluene	300 x 10 ⁻⁹	BD
2,4,6-Trinitrotoluene	46 x 10 ⁻⁹	140 x 10 ⁻⁹
2-Nitronaphthalene	15 x 10 ⁻⁹	BD
N-Nitrosodiphenylamine	29 x 10 ⁻⁹	BD
1,3,5-Trinitrobenzene	BD	BD
2-Nitrodiphenylamine	N/A ^d	BD
1-Nitropyrene	59 x 10 ⁻⁹	BD
Naphthalene	12 x 10 ⁻⁹	1800 x 10 ⁻⁹
Benz[a]anthracene	66 x 10 ⁻⁹	320 x 10 ⁻⁹
Benzo[a]pyrene	310 x 10 ⁻⁹	BD
Pyrene	N/A	19 x 10 ⁻⁹
Phenol	12000 x 10 ⁻⁹	BD
Dibenzofuran	60 x 10 ⁻⁹	190 x 10 ⁻⁹
Diphenylamine	25 x 10 ⁻⁹	BD

^aEmission factors are expressed in terms of 10⁻⁹ for ease of comparison, e.g., 200 x 10⁻⁹ is equivalent to 0.000000200.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection limits.

^cBelow detection limit.

^dNot included on analyte list for analysis.

b. In most cases semivolatile compounds detected during these tests include the parent compound, 2,4,6-TNT, as well as the 2,4- and 2,6-dinitrotoluene compounds. The compounds occurring in the highest concentrations are typically phenol and naphthalene, with EFs about 0.000001. Most of the other detected compounds are observed at levels 10-fold to 1000-fold lower than those for phenol and naphthalene.

c. An examination of semivolatile results for the suspended tests reveals that the emission levels do not change appreciably from those measured in the *surface* tests. This is an important observation and stands in contrast to the lower EFs for such species as CO and VOC seen in the

suspended TNT tests. Above-ground elevation of the bulk explosive prior to detonation does not appear to have a significant effect on the production of semivolatile organic compounds.

4.2.1.2 Soil

4.2.1.2.1 Ejecta.

Ejecta soil is the soil displaced at the point of a *surface* detonation and redeposited in the crater, in the berm around the crater, and within a few meters of the crater. The volume of the displaced soil was estimated using Equation 4.2, paragraph 4.1.3.3. The calculated crater volume for TNT tests are shown in Table 4.2.8. The volume of the displaced soil varied from 12 to 42 m³. The calculated weight of the soil, based on a density of 2.5 g/cc, varied from 29 to 105 metric tons, with a mean of 56 metric tons. This loose soil was sampled, and the semivolatile organics remaining after the detonation were identified and quantified. Background soil samples of the sites were taken prior to the detonations to provide a baseline concentration level of semivolatile organics in the local soil.

Table 4.2.8 OB/OD Detonation Crater Dimension, Volume, and Weight of Displaced Soil.

Location	Rim Opening (m)	Depth (m)	Volume (m³)	Weight of Soil (kg)	Average Weight (kg)
TNT Surface Detonations-Phase B					56066
1	5.6	2.1	30.71	76777	
2	4.9	1.7	18.60	46503	
3	5.3	1.3	15.49	38726	
4	5.0	1.8	20.73	51813	
5	6.5	2.2	42.08	105192	
6	ND ^a	1.9	ND	ND	
7	ND	1.4	ND	ND	
TNT Surface Detonations-Phase C					
C1	4.3	1.4	11.60	29005	
C2	4.6	1.6	15.44	38600	
C3	6.7	1.8	34.78	86961	
C4	4.5	1.7	16.09	40228	
C5	ND	ND	ND	ND	
C6	4.3	1.7	14.92	37290	
C0	5.3	2.0	26.25	65627	

^aND - no data.

a. Phase A. Soil sampling was accomplished to develop and refine field soil collection methods and the chemical extraction/assay procedures. The data are summarized in Table 4.2.9.

Table 4.2.9 Summary of Phase A Pretest and Ejecta Soil Samples for Semivolatile Organics.

Source of Sample	Compounds Found ^a	Concentration Range (ng/kg) ^b
Pretest 12-ft core	None	BD ^c
Pretest 15-cm core	2,4-Dinitrotoluene	0.58 to 1.2
	2,6-Dinitrotoluene	BD to 2.7
	2-Nitronaphthalene	2.3 to 2.9
Ejecta	2,4-Dinitrotoluene	68 to 170
	2,6-Dinitrotoluene	23 to 35
	2,4,6-Trinitrotoluene	300 to 4400
	2-Nitronaphthalene	1.1 to 4.9
	1,3,5-Trinitrobenzene	BD to 160
	Naphthalene	BD to 1200
Posttest 15-cm core	2,4-Dinitrotoluene	30
	2,6-Dinitrotoluene	BD
	2,4,6-Trinitrotoluene	1500
	2-Nitronaphthalene	1.1
	1,3,5-Trinitrobenzene	11
	Naphthalene	BD
Pan-composite	2,4-Dinitrotoluene	160
	2,6-Dinitrotoluene	140
	2,4,6-Trinitrotoluene	190
	2-Nitronaphthalene	2.7
	1,3,5-Trinitrobenzene	240
	Naphthalene	2300

^aSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^bRepresents ng of analyte per kg of soil.

^cBelow detection limit.

b. Phases B and C.

(1) Background samples were taken at all detonation sites. Although sampling procedures differed somewhat between phases B and C, (depth of core, number of cores, and the compositing of samples), all samples were from an area at DPG considered uncontaminated from previous explosive detonations. The ejecta sampling at each site on Phases B and C were similar, although

compositing of samples differed between the two phases. The summary data are shown in Table 4.2.10. The analytes which showed increased concentrations (above concentration levels in the pretest soil) in the ejecta soil after detonation were 2,4,6-trinitrotoluene, 1,3,5-trinitrobenzene, benz[a]anthracene, pyrene, and phenol.

Table 4.2.10 Summary of Semivolatile Organic Concentrations from Phases B and C Pretest and Ejecta Soil Samples, Based on the Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range ($\mu\text{g/kg}$) ^c	Geometric Mean ^d ($\mu\text{g/kg}$)
	Total	AD ^a			
Pretest	10	7	2,4-Dinitrotoluene	BD ^e to 1.6	0.87
	10	5	2,6-Dinitrotoluene	BD to 9.3	5.0
	10	9	2,4,6-Trinitrotoluene	BD to 24	1.0
	10	8	2-Nitronaphthalene	BD to 1.6	0.33
	10	2	N-Nitrosodiphenylamine	BD to 0.19	0.020
	10	10	Naphthalene	0.016 to 4.8	0.89
	10	9	Benz[a]anthracene	BD to 0.39	0.21
	10	10	Pyrene	0.026 to 2.2	0.10
	10	10	Dibenzofuran	0.007 to 1.6	0.21
	10	2	Diphenylamine	BD to 0.55	0.40
Ejecta	13	9	2,4-Dinitrotoluene	BD to 8.0	1.3
	13	10	2,6-Dinitrotoluene	BD to 2.3	0.70
	13	13	2,4,6-Trinitrotoluene	1.7 to 360	23
	13	8	2-Nitronaphthalene	BD to 1.8	0.27
	13	6	N-Nitrosodiphenylamine	BD to 1.1	0.18
	13	8	1,3,5-Trinitrobenzene	BD to 39	0.97
	13	1	1-Nitropyrene	BD to 1.2	1.2
	13	13	Naphthalene	0.028 to 210	7.0
	13	10	Benz[a]anthracene	BD to 11	1.3
	13	12	Pyrene	BD to 53	2.4
	13	1	Phenol	BD to 69	69
	13	10	Dibenzofuran	BD to 18	0.59
	13	2	Diphenylamine	BD to 0.79	0.67

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed only from the values above the detection limit.

^eBelow detection limit.

4.2.1.2.2 Fallout

Fallout for these OB/OD tests is defined as the particulate material deposited beyond the ejecta area. On the Phase A trials, samples were collected to verify and refine the methodologies of sample placement, sample type, sample handling, and laboratory extraction and assay. The Phase B and C tests were designed to characterize the resulting soil fallout pattern and the amount of species deposited on the soil. The background and ejecta data were included along with the fallout data prior to performing the ANOVA; this permitted the comparison of background, ejecta, 50-meter fallout, and 100-meter fallout soil data.

a. Surface TNT Detonations, Phase A.

Fallout was sampled with both a 1-m² pan and a 15-cm depth core sampler at each sampling point. The data were valuable for identifying analytes present in the soil before and after detonation and for refining sampling technology; however, the close proximity of the detonations permitted overlap of fallout and thus rendered the data useless for characterizing a single detonation. A summary of the semivolatile organics detected, and the concentration for the two types of samples are shown in Table 4.2.11.

Table 4.2.11 Summary of Semivolatile Analyte Concentrations Detected in Soil Samples in Phase A TNT Detonations.

Analyte	Concentration (ng/kg) ^a	
	Soil Core	Fallout Pan
2,4-Dinitrotoluene	32	170
2,6-Dinitrotoluene	BD ^b	140
2,4,6-Trinitrotoluene	1600	190
2-Nitronaphthalene	1.2	2.6
1,3,5-Trinitrobenzene	12	240
Naphthalene	BD	2400

^aRepresents ng of analyte per kg of soil.

^bBelow detection limit.

(1) The results indicate the following:

(a) Chemical extraction and analysis of semivolatile analyte compounds is possible,

(b) The pan samples are more representative of the fallout soil than the 15-cm cores, which are almost entirely samples of undisturbed soil. The pan samples represent a deposition area of 1 m², whereas the 5-cm diameter core represents an area of 0.002 m²,

(c) The pans must be located at least 50 meters from detonation points to avoid damage by the blast wave.

b. Surface TNT Detonations, Phases B and C.

Fallout sampling for a *surface* detonation was done with 1-m² pans on all trials. On the Phase B ORI and all Phase C trials, pans were placed on the 50-, 100-, 150-, and 200-meter circles. On other *surface* detonations, sampling was only on the 50-, and 100-meter circles.

(1) The analyte concentration data from the 50- and 100-meter sampling circles for the *surface* detonations are summarized in Table 4.2.12a. The analyte concentration data for the 150- and 200-meter sampling circles are summarized in Table 4.2.12b. The weight of sample available for assay after combining the fallout pan samples (six 1-m² samples) varied from 3.6 to 35 grams at 150 meters and 1 to 4.9 grams at 200 meters from the detonation. The analytes 2,4-dinitrotoluene, 2,4,6-trinitrotoluene, 1,3,5-trinitrobenzene, benz[a]anthracene, and pyrene were detected above background levels on the 50-meter circle. The analytes 2,4-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, naphthalene, benz[a]anthracene, pyrene, and dibenzofuran were detected above background levels on the 100-meter circle. The analytes identified on the 150-meter and 200-meter circles were the same analytes identified by soil samples from the ejecta, and fallout at 50 and 100 meters.

Table 4.2.12a Summary of Semivolatile Organic Concentrations from Phases B and C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range ($\mu\text{g/kg}$) ^c	Geometric Mean ^d ($\mu\text{g/kg}$)
	Total	AD ^a			
50-m circle	7	4	2,4-Dinitrotoluene	BD ^e to 32	4.0
	7	5	2,6-Dinitrotoluene	BD to 7.8	0.77
	7	7	2,4,6-Trinitrotoluene	6.8 to 45	13
	7	4	2-Nitronaphthalene	BD to 2.6	0.43
	7	3	1,3,5-Trinitrobenzene	BD to 0.89	0.28
	7	1	N-Nitrosodiphenylamine	BD to 0.069	0.069
	7	7	Naphthalene	0.50 to 74	6.0
	7	5	Benz[a]anthracene	BD to 6.4	1.3
	7	6	Pyrene	BD to 36	1.7
	7	5	Dibenzofuran	BD to 2.3	0.73
100-m circle	7	4	2,4-Dinitrotoluene	BD to 35	9.2
	7	4	2,6-Dinitrotoluene	BD to 21	3.0
	7	7	2,4,6-Trinitrotoluene	11 to 310	75
	7	2	2-Nitronaphthalene	BD to 47	8.7
	7	3	1,3,5-Trinitrobenzene	BD to 19	5.2
	7	7	Naphthalene	0.30 to 220	21
	7	6	Benz[a]anthracene	BD to 51	5.6
	7	2	Benzo[a]pyrene	BD to 8.5	6.4
	7	6	Pyrene	BD to 21	4.7
	7	4	Dibenzofuran	BD to 29	5.2
	7	1	Diphenylamine	BD to 5.4	5.4

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

Table 4.2.12b Summary of Semivolatile Organic Concentrations from Phases B and C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range ($\mu\text{g/kg}$) ^c	Geometric Mean ^d ($\mu\text{g/kg}$)
	Total	AD ^e			
150-m circle	3	1	2,6-Dinitrotoluene	BD ^e to 2.1	2.1
	3	2	2,4,6-Trinitrotoluene	BD to 35	26
	3	2	Naphthalene	BD to 19	11
	3	1	Benz[a]anthracene	BD to 1.9	1.9
	3	2	Benzo[a]pyrene	BD to 9.1	7.8
	3	1	Pyrene	BD to 10	10
	3	2	Diphenylamine	BD to 97	33
200-m circle	3	2	2,4,6-Trinitrotoluene	BD to 680	110
	3	1	Naphthalene	BD to 510	510
	3	1	Benz[a]anthracene	BD to 87	87
	3	1	Pyrene	BD to 88	88
	3	3	Diphenylamine	5.7 to 97	24

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

(2) The Duncan's multiple-range test comparing the ejecta sample results with the fallout sample results for the semivolatile organics shows the following:

(a) The ejecta analyte concentration means were not different from the 50-meter concentration means.

(b) The 100-meter concentration means for 2,4-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, and dibenzofuran were larger than the ejecta concentration means.

(3) This increase in concentration of the semivolatile analytes on the fallout soil at greater distance from the detonation may be a function of particle size. The increased surface area per volume of particle that results with the smaller particles provides more surface area for absorption of the analyte. The results of these tests show that analytes in the 200-, 150-, and 100-meter fallout

samples were more concentrated than in the 50-meter fallout samples. The results did not show the 50-meter analyte concentrations to be greater than the ejecta concentration means. A probable explanation of this is that soil chunks are propelled as far as 50-meters and the sample is a composite of a wide range of particle sizes, including the larger chunks whose interior volume is not exposed to detonation products. This is in contrast to the fallout samples at greater distances, which consist of smaller particles.

(4) Relationship of Mass of Analyte to Fallout Area. The mass of analyte collected was compared to the total sampling area of the fallout pans making up the sample. The data are summarized in Tables 4.2.13a and 4.2.13b. These data are useful in estimating the amount of an analyte that is deposited on the terrain as a function of distance from the source.

Table 4.2.13a Summary of Semivolatile Organic Concentrations from Phases B and C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range ($\mu\text{g}/\text{m}^2$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{m}^2$)
	Total	AD ^e			
50-m circle	7	4	2,4-Dinitrotoluene	BD ^e to 3.8	0.47
	7	5	2,6-Dinitrotoluene	BD to 0.48	0.080
	7	7	2,4,6-Trinitrotoluene	0.48 to 5.3	1.2
	7	4	2-Nitronaphthalene	BD to 0.25	0.045
	7	1	N-Nitrosodiphenylamine	BD to 0.008	0.008
	7	3	1,3,5-Trinitrobenzene	BD to 0.063	0.026
	7	7	Naphthalene	0.047 to 8.7	0.59
	7	5	Benz[a]anthracene	BD to 0.73	0.14
	7	6	Pyrene	BD to 4.2	0.18
	7	5	Dibenzofuran	BD to 0.24	0.081
100-m circle	7	4	2,4-Dinitrotoluene	BD to 0.29	0.15
	7	4	2,6-Dinitrotoluene	BD to 0.18	0.047
	7	7	2,4,6-Trinitrotoluene	0.045 to 2.7	0.88
	7	2	2-Nitronaphthalene	BD to 0.38	0.14
	7	3	1,3,5-Trinitrobenzene	BD to 0.16	0.052
	7	7	Naphthalene	0.090 to 2.1	0.24
	7	6	Benz[a]anthracene	BD to 0.48	0.064
	7	2	Benzo[a]pyrene	BD to 0.072	0.69
	7	6	Pyrene	BD to 0.60	0.054
	7	4	Dibenzofuran	BD to 0.30	0.086
	7	1	Diphenylamine	BD to 0.021	0.021

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per m^2 of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

Table 4.2.13b Summary of Semivolatile Organic Concentrations from Phases B and C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range ($\mu\text{g}/\text{m}^2$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{m}^2$)
	Total	AD ^a			
150-m circle	3	1	2,6-Dinitrotoluene	BD ^e to 0.012	0.012
	3	2	2,4,6-Trinitrotoluene	BD to 0.20	0.060
	3	2	Naphthalene	BD to 0.11	0.025
	3	1	Benz[a]anthracene	BD to 0.011	0.011
	3	2	Benzo[a]pyrene	BD to 0.038	0.018
	3	1	Pyrene	BD to 0.058	0.058
	3	2	Diphenylamine	BD to 0.029	0.017
200-m circle	3	2	2,4,6-Trinitrotoluene	BD to 0.11	0.041
	3	1	Naphthalene	BD to 0.420	0.420
	3	1	Benz[a]anthracene	BD to 0.071	0.071
	3	1	Pyrene	BD to 0.072	0.072
	3	3	Diphenylamine	0.0047 to 0.016	0.0083

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per m^2 of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

c. Suspended TNT Detonations, Phase B.

The Phase B suspended detonation sampling was accomplished by taking a 15-cm diameter core to a depth of 2.5 cm on the 1-, 2-, 4-, 8-, and 16-meter sampling circles. The soil was sampled prior to the suspended detonation to establish background concentration levels for the semivolatiles. These samples were taken horizontally out to 16 meters from a point on the ground directly under the suspended TNT. The same fallout sampling points and procedures were used for the post detonation samples. An ANOVA comparing the means from each analyte for the background, 1-, 2-, 4-, 8-, and 16-meter samples detected no significant differences in the level of analyte. The data from the post detonation, 1-, 2-, 4-, 8-, and 16-meter samples, were combined for the summary in Table 4.2.14.

Table 4.2.14 Summary of Semivolatile Organic Concentrations from Phase B TNT Suspended Detonation Soil Samples.

Source of Sample	Number of Observations		Analyte ^b	Concentration Range (µg/kg) ^c	Geometric Mean ^d (µg/kg)
	Total	AD ^a			
Pretest	7	7	2,4-Dinitrotoluene	0.16 to 9.5	0.62
	7	7	2,6-Dinitrotoluene	0.012 to 1.3	0.08
	7	7	2,4,6-Trinitrotoluene	1.9 to 1200	33
	7	2	2-Nitronaphthalene	BD ^e to 0.10	0.04
	7	2	N-Nitrosodiphenylamine	BD to 0.30	0.27
	7	6	1,3,5-Trinitrobenzene	BD to 78	0.41
	7	7	Naphthalene	1.5 to 27	8.8
	7	7	Benz[a]anthracene	0.016 to 1.9	0.29
	7	7	Pyrene	.0090 to 2.1	1.1
	7	7	Dibenzofuran	.034 to 0.51	0.22
	7	4	Diphenylamine	BD to 0.10	0.023
Posttest	20	20	2,4-Dinitrotoluene	0.02 to 13	0.93
	20	18	2,6-Dinitrotoluene	BD to 3.1	0.65
	20	20	2,4,6-Trinitrotoluene	3.3 to 1300	25
	20	13	2-Nitronaphthalene	BD to 1.1	0.12
	20	7	N-Nitrosodiphenylamine	BD to 2.8	0.41
	20	15	1,3,5-Trinitrobenzene	BD to 17	0.63
	20	20	Naphthalene	1.4 to 86	13
	20	16	Benz[a]anthracene	BD to 4.0	0.43
	20	19	Pyrene	BD to 7.7	1.7
	20	2	Phenol	BD to 1.8	55
	20	19	Dibenzofuran	BD to 31	0.55
	20	12	Diphenylamine	BD to 0.14	0.057

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents µg of analyte per kg of soil.

^dGeometric means were computed only from the values above detection limit.

^eBelow detection limit.

4.2.1.2.3 Estimates of Total Deposition.

The methodologies developed and refined for collection of samples and analyses of data during the OB/OD testing are useful in arriving at estimates of soil deposition of emissions from munitions to be disposed of in the demilitarization inventory. The results from the detonation of approximately 1 metric ton of bulk TNT and the resulting deposition of 2,4-dinitrotoluene are used here as an example. Table 4.2.15 lists the maximum values for 2,4-dinitrotoluene concentration from the OB/OD TNT detonations that would be of use in an assessment of environmental impact.

Table 4.2.15 Summary of Fallout and 2,4-Dinitrotoluene Concentration by Weight and Area

Concentration	Back-ground	Ejecta	50-m Circle	100-m Circle	150-m Circle	200-m Circle
Fallout (grams of soil/m ² of terrain)	NA ^a	NA	80	8.9	2.4	0.42
Geometric mean (μg of analyte/kg of soil)	0.87	1.3	4	9.2	BD ^b	BD
Maximum (μg/kg)	1.6	8.0	32	35	BD	BD
Geometric mean (μg of analyte/m ² of terrain)	NA	NA	0.47	0.15	BD	BD
Maximum (μg/m ²)	NA	NA	3.8	0.29	BD	BD

^aNot applicable.

^bBelow detection limit.

a. For example, the data above can be used to determine the maximum mass of residual 2,4-dinitrotoluene that would be expected from a 1-metric-ton detonation of TNT. Using the maximum crater soil weight given in Table 4.2.8 (105 metric tons) and the maximum concentration for 2,4-dinitrotoluene at the 100-meter circle given in Table 4.2.15 (35 μg/kg), the calculated total 2,4-dinitrotoluene soil deposition from a 1-metric-ton TNT detonation is 3.7 grams. This is a conservative estimate, because all the ejecta soil is considered as contaminated at this level, whereas if the ejecta concentration value is used, it would be concluded that no 2,4-dinitrotoluene resulted from the detonation. The mean ejecta 2,4-dinitrotoluene concentration (1.3 μg/kg) does not significantly differ from the mean background concentration level at that test site (0.87 μg/kg).

b. A second example may be used to estimate the 2,4-dinitrotoluene fallout from a 1-metric-ton TNT detonation. This can be approximated by using the deposition concentration (μg of analyte per m^2 of terrain) multiplied by an assigned deposition area at each sampled distance. This is shown in Table 4.2.16 with the total amount of 2,4-dinitrotoluene fallout estimated at 76 mg. A similar calculation using the measured analyte concentration expressed in μg of analyte per kg of soil, multiplied by the mass of fallout soil in the deposition area, yields a total amount of 2,4-dinitrotoluene of 55 mg. This means that about 2.0 percent of the 3.7 gram total 2,4-dinitrotoluene soil deposition was recovered as fallout within 225 meters of the detonation site. In other words, about 98 percent of the total 2,4-dinitrotoluene residues are in the immediate vicinity of the crater in the soil ejecta.

Table 4.2.16 Concentration and Deposition Area Used to Determine Fallout Amount for 2,4-Dinitrotoluene.

Distance Interval (m)	Deposition Area (m^2)	Concentration ($\mu\text{g}/\text{m}^2$)	Fallout Amount (mg)
0 to 75	17,671	3.8	67
75 to 125	31,416	0.29	9
125 to 175	47,124	BD*	0
175 to 225	62,832	BD	0
Total =			76

*Below detection limit.

c. The results reveal some important implications for future characterization of OB/OD demilitarization of explosive munitions. First, crater mass and fallout mass at various distances should be well documented. Along with these weight measurements, a concentration of analytes in the fallout soil is required. It is suggested that this can be accomplished with chemical analysis of soil at 100 meters; this distance is suggested because it provided sufficient sample size for extraction and it was also free of clods. The analyte concentration at 100 meters would be used to characterize the ejecta soil and fallout soil at all sampling points based on the mass of soil collected. If implemented, these changes would result in less chemical analyses, thus reducing the cost of testing.

4.2.2 Composition B Test - Phase C

4.2.2.1 Air Emissions

4.2.2.1.1 Gases

a. Gas EFs measured during the six 907-kg composition B detonations are statistically summarized in Table 4.2.17. Carbon dioxide EFs range from 0.86 to 0.87. An average value of 0.87 compares with a theoretical CO₂ EF of 0.92, assuming 100-percent conversion of explosive carbon to CO₂. This corresponds to a detonation efficiency of about 0.95. Although the oxygen balance of composition B at -53 percent is higher than that of TNT, the detonation efficiency for a *surface* detonation is about the same. From this observation it appears that the oxygen balance of the explosive molecule does not appear to play a significant role in the observed carbon conversion efficiency in the detonation process. The entrainment of ambient air into the fireball provides additional oxygen to provide the high carbon-conversion efficiencies observed.

Table 4.2.17 Gas Emission Factors for Composition-B Surface Detonations.

Species	Emission Factor (g/g)
CO ₂ - min	0.86
CO ₂ - max	0.87
CO ₂ - avg	0.87
CO - min	0.026
CO - max	0.037
CO - avg	0.031
NO - min	BD
NO - max	1.8×10^{-3}
NO - avg	0.8×10^{-3}
NO ₂ - min	0.009×10^{-3}
NO ₂ - max	2.3×10^{-3}
NO ₂ - avg	1.0×10^{-3}

b. Carbon monoxide EFs are correspondingly low, ranging from 0.026 to 0.037, with an average of 0.031. Emission factors measured for NO and NO₂ are in the vicinity of 1×10^{-3} . In both cases, the measured levels are comparable to those measured for TNT.

4.2.2.1.2 Particulates

Particulate mass concentrations measured during multiple aircraft passes through the detonation clouds from the composition B tests are summarized in Table 4.2.18. Cloud particle concentrations from the two three-detonation trials were about 200 mg/m³. The carbon content of the particulate samples was not measured in this test series; however, on the basis of earlier phase B TNT tests, virtually all the collected particulates are suspended soil.

Table 4.2.18 Average Particulate Matter Concentrations Measured During Multiple Aircraft Sampling Passes of Composition-B Detonation Clouds.

Test Event	Particulate Matter Concentration (mg/m ³)
Composition-B - first 3-detonation series	218
Composition-B - second 3-detonation series	191

4.2.2.1.3 Volatile Organic Compounds

VOC EFs for the composition B *surface* detonations as sampled with 6-L canisters and followed by gas chromatographic analysis are summarized in Table 4.2.19. The results are very similar to those observed from the TNT tests, with relatively low methane and TNMHC releases. The toxic VOC category as represented by benzene is similarly low, with an average EF of about 0.000062.

Table 4.2.19 Volatile Organic Compound Emission Factors Measured for the Composition-B Detonation Tests.

Species	Emission Factor (g/g)
CH ₄ - min	0.4 x 10 ⁻³
CH ₄ - max	0.8 x 10 ⁻³
CH ₄ - avg	0.6 x 10 ⁻³
TNMHC - min	0.5 x 10 ⁻³
TNMHC - max	2.3 x 10 ⁻³
TNMHC - avg	1.2 x 10 ⁻³
Benzene - min	29 x 10 ⁻⁶
Benzene - max	86 x 10 ⁻⁶
Benzene - avg	62 x 10 ⁻⁶

4.2.2.1.4 Semivolatile Organics (Exotics)

Emission factors for the semivolatile organic target compounds are given in Table 4.2.20 for the Phase C surface detonation of composition B, which is a mixture of TNT and RDX. The values shown in the table are the maximum values obtained from two separate trials each consisting of three detonations in series. Analyses for the semivolatile target analytes were done by SFC-MS which allows the determination of thermally labile compounds such as the parent explosive RDX, which would otherwise decompose during separation by conventional gas chromatography. The EFs for the target analytes are all observed at less than the part per million (10⁻⁶) level. The highest EFs observed were for 2,4-dinitrotoluene and naphthalene at levels of about 4 x 10⁻⁷. Next highest EFs were 2,4,6-trinitrotoluene, and pyrene at a level of about 2 x 10⁻⁷. In this test series the parent compound RDX was not seen although it accounts for about 40 percent of the mass of the composition B explosive. The remainder of the target analytes were either not detected or observed at lower levels. To place these EFs into perspective, consider that about 1 gram of TNT parent compound (accounts for about 60 percent of the composition B mass), would be released into the detonation cloud following the detonation of a metric ton of composition B, assuming that the TNT EF is 1 x 10⁻⁶. If a stable detonation cloud volume of 10⁶ cubic meters is assumed, the elevated

cloud concentration of TNT would be 1 μg per cubic meter. A further dilution of about 4 or 5 orders of magnitude would typically result following downwind movement of the cloud prior to its ground contact. Downwind ground-level concentrations of TNT would then be in the tens or hundreds of pg (10^{-12} g) per cubic meter of air.

Table 4.2.20 Maximum Semivolatile Organic Emission Factors Measured for Surface Composition B Detonations^a.

Species ^b	Emission Factor (g/g)
2,4-Dinitrotoluene	450×10^{-9}
2,6-Dinitrotoluene	24×10^{-9}
2,4,6-Trinitrotoluene	250×10^{-9}
2-Nitronaphthalene	86×10^{-9}
N-Nitrosodiphenylamine	36×10^{-9}
1,3,5-Trinitrobenzene	59×10^{-9}
2-Nitrodiphenylamine	72×10^{-9}
1-Nitropyrene	56×10^{-9}
RDX	BD ^c
Naphthalene	420×10^{-9}
Benz[a]anthracene	7.4×10^{-9}
Benzo[a]pyrene	14×10^{-9}
Pyrene	210×10^{-9}
Phenol	... ^d
Dibenzofuran	BD
Diphenylamine	66×10^{-9}

^aEmission factors are expressed in terms of 10^{-9} for ease of comparison, e.g., 450×10^{-9} is equivalent to 0.000000450.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels.

^cBelow detection limit.

^d---Phenol was lost in the extraction of the semivolatiles.

4.2.2.2 Soil

4.2.2.2.1 Ejecta

a. Ejecta soil is the soil displaced at the point of a *surface* detonation and redeposited in the crater, in the berm around the crater, and within a few meters of the crater. The volume of the

displaced soil was estimated, using Equation 4.2, paragraph 4.1.3.3. The calculated results are given in Table 4.2.21. The volume of the displaced soil varied from 22 to 28 m³. The calculated weight of this soil, based on a density of 2.5 g/cc, varied from 55 to 70 metric tons, with a mean of 64 metric tons. This loose soil was sampled, and the semivolatile organics remaining after the detonation were identified and quantified.

Table 4.2.21 OB/OD Detonation Crater Dimension, Volume, and Weight of Displaced Soil for Composition B.

Location	Rim Opening (m)	Depth (m)	Volume (m ³)	Weight of Soil (kg)	Average Weight (kg)
Composition B					
B0	5.0	2.0	23.82	59559	64056
B1	ND ^a	ND	ND	ND	
B2	5.0	1.9	22.24	55611	
B3	5.5	2.0	27.95	69868	
B4	5.0	2.0	23.82	59559	
B5	ND	ND	ND	ND	
B6	5.5	2.0	27.95	69868	
D0	5.5	2.0	27.95	69868	

^aND - no data.

b. Background samples were taken at all detonation sites. All detonation sites were located in an area at DPG considered uncontaminated from previous explosive detonations. The pretest (background) and ejecta summary data are given in Table 4.2.22. The analyte which showed increased concentration (above concentration levels detected in the pretest soil) in the ejecta soil after detonation was 2,4,6-trinitrotoluene.

Table 4.2.22 Composition B, Summary of Semivolatile Organic Concentrations from Phase C Pretest and Ejecta Soil Samples, Based on the Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g/kg}$) ^c	Geometric Mean ^d ($\mu\text{g/kg}$)
	Total	AD ^e			
Pretest	3	3	2,4-Dinitrotoluene	1.3 to 6.4	3.7
	3	3	2,6-Dinitrotoluene	0.13 to 0.24	0.19
	3	3	2,4,6-Trinitrotoluene	0.58 to 2.3	1.2
	3	3	2-Nitronaphthalene	0.075 to 0.24	0.16
		2	N-Nitrosodiphenylamine	BD ^e to 1.3	0.68
	3	2	1,3,5-Trinitrobenzene	BD to 0.87	0.25
	3	2	2-Nitrodiphenylamine	BD to 0.21	0.14
	3	1	Naphthalene	BD to 0.16	0.16
	3	2	Benz[a]anthracene	BD to 1.2	0.93
	3	3	Pyrene	0.14 to 1.2	0.40
	3	3	Diphenylamine	0.11 to 0.36	0.22
Ejecta	3	3	2,4-Dinitrotoluene	10 to 17	14
	3	3	2,6-Dinitrotoluene	0.57 to 1.0	0.79
	3	3	2,4,6-Trinitrotoluene	12 to 14	13
	3	3	2-Nitronaphthalene	0.078 to 0.39	0.16
	3	1	N-Nitrosodiphenylamine	BD to 0.39	0.39
	3	3	1,3,5-Trinitrobenzene	0.14 to 0.39	0.22
	3	2	2-Nitrodiphenylamine	BD to 0.60	0.24
	3	1	1-Nitropyrene	BD to 0.14	0.14
	3	3	Naphthalene	3.4 to 13	6.9
	3	2	Benz[a]anthracene	BD to 1.9	1.5
	3	1	Benzo[a]pyrene	BD to 0.55	0.55
	3	3	Pyrene	1.4 to 4.5	2.7
	3	2	Dibenzofuran	BD to 1.6	1.4
	3	2	Diphenylamine	BD to 1.6	1.4

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed only from the values above the detection limit.

^eBelow detection limit.

4.2.2.2.2 Fallout

a. Fallout for the OB/OD thermal treatment testing is defined as the particulate material deposited beyond the ejecta area. The Phase C testing was conducted partly to characterize the resulting soil fallout pattern and amount of species deposited on the soil. The background and ejecta data were included along with the fallout data, prior to performing the ANOVA.

b. Phase C . Fallout for a *surface* detonation was sampled with 1-m² pans placed on the 50-, 100-, 150-, and 200-meter circles.

(1) The analyte concentration data from the 50- and 100-meter sampling circles for the *surface* detonations are summarized in Table 4.2.23a. The analyte concentration data for the 150- and 200-meter sampling circles are presented in Table 4.2.23b. The analytes detected above background levels on the 50-meter circle were 2,4-dinitrotoluene, and 2,4,6-trinitrotoluene. The analytes above background levels on the 100-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, pyrene, and diphenylamine. The analytes detected above background levels on the 150-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 2-nitrodiphenylamine, pyrene, and diphenylamine. The analytes detected above background levels on the 200-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, naphthalene, benz[a]anthracene, pyrene, and diphenylamine. Dibenzofuran was not found in the background sample but was found in some of the ejecta and fallout pan samples.

Table 4.2.23a Composition B, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^a			
50-m circle	3	3	2,4-Dinitrotoluene	12 to 150	52
	3	1	2,6-Dinitrotoluene	BD ^e to 0.67	0.67
	3	3	2,4,6-Trinitrotoluene	11 to 220	39
	3	2	2-Nitronaphthalene	BD to 0.47	0.25
	3	3	1,3,5-Trinitrobenzene	0.26 to 1.6	0.50
	3	1	1-Nitropyrene	BD to 1.1	1.1
	3	3	Naphthalene	0.58 to 1.5	0.47
	3	2	Pyrene	BD to 1.4	0.76
	3	3	Dibenzofuran	0.36 to 3.1	1.0
100-m circle	3	3	2,4-Dinitrotoluene	640 to 1800	1230
	3	3	2,6-Dinitrotoluene	2.5 to 27	7.5
	3	3	2,4,6-Trinitrotoluene	47 to 92	69
	3	3	2-Nitronaphthalene	1.9 to 7.5	3.1
	3	3	1,3,5-Trinitrobenzene	0.062 to 9.8	0.96
	3	1	2-Nitrodiphenylamine	BD to 1.1	1.1
	3	1	1-Nitropyrene	BD to 1.0	1.0
	3	1	Naphthalene	BD to 8.7	8.7
	3	2	Benz[a]anthracene	BD to 8.6	6.5
	3	3	Pyrene	2.3 to 9.8	6.0
	3	1	Dibenzofuran	BD to 6.2	6.2
	3	3	Diphenylamine	1.3 to 6.6	3.4

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

Table 4.2.23b Composition B, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^a			
150-m circle	3	3	2,4-Dinitrotoluene	360 to 5600	1200
	3	3	2,6-Dinitrotoluene	5.1 to 49	18
	3	3	2,4,6-Trinitrotoluene	13 to 330	81
	3	3	2-Nitronaphthalene	0.77 to 21	4.1
	3	2	1,3,5-Trinitrobenzene	BD ^e to 4.9	2.3
	3	3	2-Nitrodiphenylamine	1.3 to 17	5.9
	3	1	1-Nitropyrene	BD to 15	15
	3	2	Naphthalene	BD to 37	8.4
	3	3	Benz[a]anthracene	0.59 to 33	5.9
	3	3	Pyrene	1.4 to 64	9.8
	3	1	Dibenzofuran	BD to 35	35
	3	3	Diphenylamine	1.0 to 33	6.9
200-m circle	3	3	2,4-Dinitrotoluene	2100 to 8900	4400
	3	3	2,6-Dinitrotoluene	79 to 330	130
	3	3	2,4,6-Trinitrotoluene	130 to 970	450
	3	3	2-Nitronaphthalene	26 to 33	29
	3	3	1,3,5-Trinitrobenzene	9.0 to 21	15
	3	3	2-Nitrodiphenylamine	8.8 to 84	29
	3	1	1-Nitropyrene	BD to 37	37
	3	3	Naphthalene	8.9 to 140	34
	3	2	Benz[a]anthracene	26 to 76	51
	3	1	Benzo[a]pyrene	BD to 32	32
	3	1	Pyrene	30 to 170	73
	3	3	Dibenzofuran	4.6 to 57	20
	3	2	Diphenylamine	BD to 130	76

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

(2) The Duncan's multiple-range test comparing the ejecta sample results with the fallout sample results for the semivolatile organics shows the following:

(a) The ejecta analyte concentration means were not different from the 50-meter concentration means.

(b) The 100-meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, and 2-nitronaphthalene were larger than the ejecta concentration means for these same compounds.

(c) The 150-meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2-nitronaphthalene, and 2-nitrodiphenylamine were larger than the ejecta concentration means for these same compounds.

(d) The 200 meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2 nitrodiphenylamine, benz[a]anthracene, pyrene, and diphenylamine were larger than the ejecta concentration means for these same compounds.

(3) This increase in concentration of the semivolatile analytes on the fallout soil at greater distance from the detonation may be a function of particle size. The increased surface area per volume of particle that results with the smaller particles provides more surface area for absorption of the analyte. The results of the OB/OD test show that analytes in the 200-, 150-, and 100-meter fallout samples were more concentrated than in the 50-meter fallout samples. The results did not show the 50-meter analyte concentrations to be greater than the ejecta concentration means. A probable explanation of this is that soil chunks are still being propelled as far as 50 meter and the sample is a composite of a wide range of particle sizes including the larger chunks whose interior volume is not exposed to detonation products. This is in contrast to the fallout samples at greater distances which consist of smaller particles.

(4) Relationship of Mass of Analyte to Fallout Area. The mass of analyte collected was compared to the total sampling area of the fallout pans making up the sample. The data is

summarized in Tables 4.2.24a and 4.2.24b. These data are useful in estimating the amount of an analyte that is deposited on the terrain as a function of distance from the source.

Table 4.2.24a Composition B, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ³) ^c	Geometric Mean ^d (ng/m ³)
	Total	AD ^a			
50-m circle	3	3	2,4-Dinitrotoluene	630 to 9200	3100
	3	1	2,6-Dinitrotoluene	BD ^e to 47	47
	3	3	2,4,6-Trinitrotoluene	680 to 15000	2300
	3	3	2-Nitronaphthalene	BD to 25	14
	3	3	1,3,5-Trinitrobenzene	14 to 110	30
	3	1	1-Nitropyrene	BD to 66	66
	3	3	Naphthalene	4.0 to 90	28
	3	2	Pyrene	BD to 95	49
	3	3	Dibenzofuran	25 to 170	62
100-m circle	3	3	2,4-Dinitrotoluene	6800 to 9700	8500
	3	3	2,6-Dinitrotoluene	27 to 160	52
	3	3	2,4,6-Trinitrotoluene	250 to 820	480
	3	3	2-Nitronaphthalene	10 to 43	21
	3	3	1,3,5-Trinitrobenzene	0.33 to 57	6.7
	3	1	2-Nitrodiphenylamine	BD to 6.0	6.0
	3	1	1-Nitropyrene	BD to 6.0	6.0
	3	1	Naphthalene	BD to 47	47
	3	2	Benz[a]anthracene	BD to 50	37
	3	3	Pyrene	25 to 57	41
	3	1	Dibenzofuran	BD to 33	33
	3	3	Diphenylamine	14 to 38	24

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

Table 4.2.24b Composition B, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ²) ^c	Geometric Mean ^d (ng/m ²)
	Total	AD ^a			
150-m circle	3	3	2,4-Dinitrotoluene	1800 to 6800	3200
	3	3	2,6-Dinitrotoluene	22 to 98	49
	3	3	2,4,6-Trinitrotoluene	150 to 270	210
	3	3	2-Nitronaphthalene	9.2 to 15	11
	3	2	1,3,5-Trinitrobenzene	BD ^e to 20	15
	3	3	2-Nitrodiphenylamine	7.7 to 25	16
	3	1	1-Nitropyrene	BD to 6.7	6.7
	3	2	Naphthalene	BD to 82	55
	3	3	Benz[a]anthracene	11 to 23	16
	3	3	Pyrene	23 to 28	26
	3	1	Dibenzofuran	BD to 16	16
	3	3	Diphenylamine	15 to 22	19
200-m circle	3	3	2,4-Dinitrotoluene	1500 to 5300	2500
	3	3	2,6-Dinitrotoluene	57 to 92	71
	3	3	2,4,6-Trinitrotoluene	145 to 630	250
	3	3	2-Nitronaphthalene	5.7 to 32	16
	3	3	1,3,5-Trinitrobenzene	3.7 to 22	8.6
	3	3	2-Nitrodiphenylamine	7.8 to 37	16
	3	1	1-Nitropyrene	BD to 42	42
	3	3	Naphthalene	10 to 28	19
	3	3	Benz[a]anthracene	11 to 85	28
	3	3	Pyrene	27 to 90	41
	3	3	Dibenzofuran	5.2 to 28	11
	3	2	Diphenylamine	BD to 150	76

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

4.2.3 Explosive D Test - Phase C

4.2.3.1 Air Emissions

4.2.3.1.1 Gases

a. Gas EFs for the six *surface* explosive D detonations are summarized in Table 4.2.25. The CO₂ EF average ranges from 0.97 to 1.00, with an average of 0.99. The theoretical EF is 1.07, assuming complete conversion of explosive carbon to CO₂. The ratio of observed carbon conversion to theoretical, or the detonation efficiency, is 0.93 and very nearly the same as all other *surface*-detonated explosives evaluated in this test series. Although the oxygen balance of explosive D at -52 percent is greater than TNT and about the same as composition B, the detonation efficiency for a *surface* detonation is about the same.

Table 4.2.25 Gas Emission Factors for Explosive-D Surface Detonations.

Species	Emission Factor (g/g)
CO ₂ - min	0.97
CO ₂ - max	1.00
CO ₂ - avg	0.99
CO - min	0.046
CO - max	0.064
CO - avg	0.053
NO - min	0.4×10^{-3}
NO - max	1.5×10^{-3}
NO - avg	0.9×10^{-3}
NO ₂ - min	0.4×10^{-3}
NO ₂ - max	1.6×10^{-3}
NO ₂ - avg	1.1×10^{-3}

b. Carbon-monoxide EFs for explosive D range from a low of 0.046 to a high of 0.064, with an average of 0.053. Nitric oxide and NO₂ EFs are in the vicinity of 0.001 and comparable to those

observed for the other explosives. The ratio of NO to NO₂ EFs for this explosive is also very nearly one.

4.2.3.1.2 Particulates

a. The particulate mass concentration in the explosive D detonation clouds as measured during multiple aircraft passes is summarized in Table 4.2.26. Cloud particle concentrations from the two trials of three-detonations each show more variability than encountered for the other explosive types, with a high concentration of about 300 and a low of 180 mg/m³. Differences in soil compaction at the various detonation sites may account for the variability noted.

Table 4.2.26 Average Particulate Matter Concentrations Measured During Multiple Aircraft Sampling Passes of Explosive-D Detonation Clouds.

Test Event	Particulate Matter Concentration (mg/m ³)
Explosive-D - First 3-detonation series	184
Explosive-D - Second 3-detonation series	315

4.2.3.1.3 Volatile Organic Compounds

Volatile organic compound EFs from the explosive D tests are given in Table 4.2.27. Average methane EFs are higher than those for composition B, by nearly a factor of ten. Emission factors for the TNMHC and benzene categories are also higher, but only by a factor of about two.

Table 4.2.27 Volatile Organic Compound Emission Factors Measured for the Explosive-D Detonation Tests.

Species	Emission Factor (g/g)
CH ₄ - min	0.7×10^{-3}
CH ₄ - max	7.7×10^{-3}
CH ₄ - avg	2.4×10^{-3}
TNMHC - min	1.2×10^{-3}
TNMHC - max	2.7×10^{-3}
TNMHC - avg	2.0×10^{-3}
Benzene - min	69×10^{-6}
Benzene - max	160×10^{-6}
Benzene - avg	110×10^{-6}

4.2.3.1.4 Semivolatile Organics (Exotics)

a. Emission factors for the semivolatile organic target compounds are given in Table 4.2.28 for the Phase C surface detonation of explosive D. The values shown in the table are the maximum values obtained from two separate tests each consisting of three detonations in series. Analysis for the semivolatile target analytes was done by SFC-MS which allows the determination of thermally unstable compounds which would otherwise decompose during separation by conventional gas chromatography. The emission factors for the target analytes are all observed at less than the part per million (10^{-6}) level. The highest emission factors observed were for 2,4-dinitrotoluene and naphthalene at levels of about 5×10^{-7} . Next highest were pyrene and dibenzofuran at a level slightly in excess of 1×10^{-7} . In this test series the parent compound picric acid is seen at a relatively low level of 5×10^{-8} . The remainder of the target elements were either not detected or observed at lower levels. To place these emission factors into perspective, consider that about 0.1 gram of picric acid would be released into the detonation cloud following the detonation of a metric ton of explosive D, if one conservatively assumes that the picric acid emission factor is 1×10^{-7} . If a stable cloud volume of 10^6 cubic meters is assumed, the elevated cloud concentration of picric acid would be about $0.1 \mu\text{g}$ per cubic meter. A further dilution of about 4 or 5 orders of magnitude would typically result following downwind movement of the cloud prior to its ground contact.

Downwind ground-level concentrations of TNT would then be in the tens or hundreds of pg (10^{-12} grams) per cubic meter of air, a vanishingly low level.

Table 4.2.28 Maximum Semivolatile Organic Emission Factors Measured for Surface Explosive D Detonations^a.

Species ^b	Emission Factor (g/g)
2,4-Dinitrotoluene	590×10^{-9}
2,6-Dinitrotoluene	80×10^{-9}
2,4,6-Trinitrotoluene	44×10^{-9}
2-Nitronaphthalene	43×10^{-9}
N-Nitrosodiphenylamine	58×10^{-9}
1,3,5-Trinitrobenzene	18×10^{-9}
2-Nitrodiphenylamine	58×10^{-9}
1-Nitropyrene	11×10^{-9}
Picric acid	50×10^{-9}
Naphthalene	630×10^{-9}
Benz[a]anthracene	19×10^{-9}
Benzo[a]pyrene	38×10^{-9}
Pyrene	180×10^{-9}
Phenol	--- ^d
Dibenzofuran	110×10^{-9}
Diphenylamine	19×10^{-9}

^aEmission factors are expressed in terms of 10^{-9} for ease of comparison, e.g., 590×10^{-9} is equivalent to 0.000000590.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels.

^cBelow detection limit.

^d---Phenol was lost in the extraction of the semivolatiles.

4.2.3.2 Soil

4.2.3.2.1 Ejecta

a. Ejecta soil is the soil displaced at the point of a *surface* detonation and redeposited in the crater, in the berm around the crater, and within a few meters of the crater. The volume of the displaced soil was estimated using Equation 4.2, paragraph 4.1.3.3. The calculated results are given in Table 4.2.29. The volume of the displaced soil varied from 37 to 53 m³. The calculated weight of this soil, based on a density of 2.5 g/cc, varied from 93 to 132 metric tons, with a mean of 114 metric tons. This loose soil was sampled, and the semivolatile organics remaining after the detonation were identified and quantified.

Table 4.2.29 OB/OD Detonation Crater Dimension, Volume, and Weight of Displaced Soil for Explosive D.

Location	Rim Opening (m)	Depth (m)	Volume (m ³)	Weight of Soil (kg)	Average Weight (kg)
Explosive D					
A1	7.5	2.0	48.37	120919	113557
A2	7.4	2.2	52.88	132211	
A3	6.7	2.1	41.87	104671	
A4	6.9	2.3	49.37	123431	
A5	6.5	2.0	37.37	93430	
A6	7.0	2.0	42.67	106683	

b. Background samples were taken at all detonation sites. All detonation sites were located in an area considered uncontaminated from previous explosive detonations. The pretest (background) and ejecta summary data are given in Table 4.2.30. The analyte which showed increased concentrations (above concentration levels in the pretest soil) in the ejecta soil after detonation was pyrene. The parent compound picric acid was found in the pretest soil sample; however it was below detection in the ejecta sample. N-nitrosodiphenylamine was found in 1 of 3 samples in the ejecta soil.

Table 4.2.30 Explosive D: Summary of Semivolatile Organic Concentrations from Phase C Pretest and Ejecta Soil Samples, Based on the Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^a			
Pretest	2	2	2,4-Dinitrotoluene	0.84 to 1.2	1.0
	2	2	2,6-Dinitrotoluene	0.074 to 0.15	0.11
	2	2	2,4,6-Trinitrotoluene	0.12 to 0.45	0.23
	2	2	2-Nitronaphthalene	0.026 to 0.24	0.080
	2	1	1,3,5-Trinitrobenzene	BD to 0.53	0.53
	2	1	2-Nitrodiphenylamine	BD to 0.29	0.29
	2	1	1-Nitropyrene	BD to 0.069	0.069
	2	1	Picric acid	BD to 0.37	0.37
	2	2	Naphthalene	1.0 to 2.6	1.6
	2	1	Benz[a]anthracene	BD to 0.98	0.98
	2	2	Pyrene	0.048 to 0.29	0.12
	2	2	Dibenzofuran	0.16 to 1.8	0.54
	2	2	Diphenylamine	0.24 to 0.32	0.28
Ejecta	3	3	2,4-Dinitrotoluene	0.48 to 1.3	0.92
	3	3	2,6-Dinitrotoluene	0.010 to 0.14	0.054
	3	3	2,4,6-Trinitrotoluene	0.52 to 7.4	1.3
	3	3	2-Nitronaphthalene	0.014 to 0.11	0.049
	3	1	N-Nitrosodiphenylamine	BD to 0.090	0.090
	3	3	1,3,5-Trinitrobenzene	0.022 to 0.14	0.043
	3	3	2-Nitrodiphenylamine	0.082 to 0.24	0.12
	3	3	1-Nitropyrene	0.0020 to 0.12	0.025
	3	3	Naphthalene	1.4 to 11	3.3
	3	2	Benz[a]anthracene	BD to 5.4	2.2
	3	1	Benzo[a]pyrene	BD to 0.67	0.67
	3	3	Pyrene	1.5 to 5.2	3.2
	3	3	Dibenzofuran	0.24 to 1.0	0.56
	3	3	Diphenylamine	0.038 to 0.26	0.15

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed only from the values above the detection limit.

^eBelow detection limit.

4.2.3.2.2 Fallout

a. Fallout for the OB/OD thermal treatment testing is defined as the particulate material deposited beyond the ejecta area. The Phase C testing was to characterize the resulting soil fallout pattern and the amount of species deposited on the soil. The background and ejecta data were included along with the fallout data prior to performing the ANOVA.

b. Phase C. Fallout from a *surface* detonation was sampled with 1-m² pans placed on the 50-, 100-, 150-, and 200-meter circles.

(1) The analyte concentration data from the 50- and 100-meter sampling circles for the *surface* detonations are summarized in Table 4.2.31a. The analyte concentration data for the 150- and 200-meter sampling circles are presented in Table 4.2.31b. The analytes detected above background levels on the 50-meter circle were 2,4,6-trinitrotoluene, and pyrene. The analytes found above background levels on the 100-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 1,3,5-trinitrobenzene, picric acid, and pyrene. The analytes detected above background levels on the 150-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, picric acid, pyrene, and diphenylamine. The analytes detected above background levels on the 200-meter circle were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, 1-nitropyrene, picric acid, naphthalene, benz[a]anthracene, pyrene, dibenzofuran and diphenylamine.

Table 4.2.31a Explosive D, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g/kg}$) ^c	Geometric Mean ^d ($\mu\text{g/kg}$)
	Total	AD ^a			
50-m circle	3	3	2,4-Dinitrotoluene	0.48 to 0.56	0.51
	3	3	2,6-Dinitrotoluene	0.059 to 0.25	0.15
	3	3	2,4,6-Trinitrotoluene	0.73 to 38	5.3
	3	1	2-Nitronaphthalene	BD ^e to 0.085	0.085
	3	3	1,3,5-Trinitrobenzene	0.041 to 0.15	0.082
	3	1	2-Nitrodiphenylamine	BD to 0.61	0.61
	3	1	1-Nitropyrene	BD to 0.081	0.081
	3	2	Picric acid	BD to 1.9	1.2
	3	3	Naphthalene	0.97 to 6.5	2.2
	3	2	Benz[a]anthracene	BD to 0.97	0.89
	3	1	Pyrene	BD to 5.9	5.9
	3	1	Diphenylamine	BD to 1.7	1.7
100-m circle	3	3	2,4-Dinitrotoluene	10 to 15	12
	3	3	2,6-Dinitrotoluene	0.60 to 1.8	1.0
	3	3	2,4,6-Trinitrotoluene	4.5 to 34	12
	3	3	2-Nitronaphthalene	0.37 to 2.9	1.1
	3	2	N-Nitrosodiphenylamine	BD to 0.96	0.83
	3	3	1,3,5-Trinitrobenzene	0.69 to 2.2	1.3
	3	2	2-Nitrodiphenylamine	BD to 1.3	0.97
	3	2	1-Nitropyrene	BD to 0.18	0.14
	3	1	Picric acid	BD to 7.1	7.1
	3	3	Naphthalene	2.7 to 9.5	6.1
	3	2	Benz[a]anthracene	BD to 0.41	0.29
	3	3	Pyrene	7.6 to 12	10
	3	1	Dibenzofuran	BD to 2.4	2.4
	3	1	Diphenylamine	BD to 1.1	1.1

^aAbove detection limit.

^bSee Table 3.16 for list containing the semivolatile organics and the detection levels in soil.

^c μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

Table 4.2.31b Explosive D, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^e			
150-m circle	3	3	2,4-Dinitrotoluene	34 to 410	82
	3	3	2,6-Dinitrotoluene	4.5 to 24	10
	3	3	2,4,6-Trinitrotoluene	11 to 73	20
	3	3	2-Nitronaphthalene	2.5 to 14	7.0
	3	3	N-Nitrosodiphenylamine	2.8 to 20	9.1
	3	3	1,3,5-Trinitrobenzene	3.5 to 17	7.1
	3	3	2-Nitrodiphenylamine	3.1 to 35	11
	3	3	1-Nitropyrene	3.2 to 16	7.8
	3	1	Picric acid	BD ^f to 18	18
	3	2	Naphthalene	BD to 29	11
	3	2	Benz[a]anthracene	BD to 5.1	3.2
	3	1	Benzo[a]pyrene	BD to 1.7	1.7
	3	2	Pyrene	BD to 65	24
	3	3	Dibenzofuran	9.2 to 130	24
	3	3	Diphenylamine	9.7 to 23	15
200-m circle	3	3	2,4-Dinitrotoluene	65 to 1300	210
	3	3	2,6-Dinitrotoluene	11 to 140	37
	3	3	2,4,6-Trinitrotoluene	15 to 460	120
	3	3	2-Nitronaphthalene	12 to 150	41
	3	3	1,3,5-Trinitrobenzene	8.1 to 100	31
	3	3	2-Nitrodiphenylamine	7.5 to 180	39
	3	3	1-Nitropyrene	4.6 to 38	18
	3	2	Picric acid	BD to 36	36
	3	3	Naphthalene	36 to 720	120
	3	1	Benz[a]anthracene	BD to 20	20
	3	1	Benzo[a]pyrene	BD to 53	53
	3	3	Pyrene	5.8 to 260	11
	3	3	Dibenzofuran	13 to 540	19
	3	2	Diphenylamine	BD to 140	10

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

(2) The Duncan's multiple-range test comparing the ejecta sample results with the fallout sample results for the semivolatile organics shows the following:

(a) The only semivolatile analyte found at 50-meter in higher concentration than in the ejecta soil was diphenylamine. Picric acid was not recovered in the ejecta soil, although it was found in the background soil from the detonation sites.

(b) The measured 100-meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, and diphenylamine were larger than the ejecta concentration means.

(c) The 150-meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2-nitronaphthalene, N-nitrosodiphenylamine, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, 1-nitropyrene, and diphenylamine were larger than the ejecta concentration means for these same compounds.

(d) The measured 200-meter concentration means for 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, 1-nitropyrene, naphthalene, dibenzofuran, and diphenylamine were larger than the ejecta concentration means for these same compounds.

(3) This increase in concentration of the semivolatile analytes on the fallout soil at greater distance from the detonation may be a function of particle size (the increased surface area per volume of particle that results with the smaller particles provides more surface area for absorption of the analyte.) The results of OE/OD test show that analytes in the 200-, 150, and 100-meter fallout samples were more concentrated than in the 50-meter fallout samples. The results did not show the 50-meter analyte concentrations to be greater than the ejecta concentration means except for diphenylamine. A probable explanation of the increased concentration of analytes with distance is that soil chunks are still being propelled as far as 50 meter and the sample is a composite of a wide range of particle sizes including the larger chunks whose interior volume is not exposed to detonation products. This is in contrast to the fallout samples at greater distances, which consist of smaller particles.

(4) Relationship of Mass of Analyte to Fallout Area. The mass of analyte collected was compared to the total sampling area of the fallout pans making up the sample. The summary of this data is shown in Tables 4.2.32a and 4.2.32b. This data are useful in estimating the amount of an analyte that is deposited on the terrain as a function of distance from the source.

Table 4.2.32a Explosive D, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ²) ^c	Geometric Mean ^d (ng/m ²)
	Total	AD ^e			
50-m circle	3	3	2,4-Dinitrotoluene	23 to 46	35
	3	3	2,6-Dinitrotoluene	4.9 to 20	10
	3	3	2,4,6-Trinitrotoluene	30 to 3600	360
	3	1	2-Nitronaphthalene	BD ^e to 3.5	3.5
	3	3	1,3,5-Trinitrobenzene	3.4 to 8.8	5.6
	3	1	2-Nitrodiphenylamine	BD to 25	25
	3	1	1-Nitropyrene	BD to 6.7	6.7
	3	2	Picric acid	BD to 180	76
	3	3	Naphthalene	81 to 270	150
	3	2	Benz[a]anthracene	BD to 91	78
	3	1	Pyrene	BD to 550	550
	3	1	Diphenylamine	BD to 160	160
100-m circle	3	3	2,4-Dinitrotoluene	67 to 110	84
	3	3	2,6-Dinitrotoluene	4.3 to 14	7.5
	3	3	2,4,6-Trinitrotoluene	37 to 220	87
	3	3	2-Nitronaphthalene	2.7 to 18	7.7
	3	2	N-Nitrosodiphenylamine	BD to 7.8	6.4
	3	3	1,3,5-Trinitrobenzene	5.0 to 14	9.6
	3	2	2-Nitrodiphenylamine	BD to 11	7.4
	3	2	1-Nitropyrene	BD to 1.3	1.1
	3	1	Picric acid	BD to 45	45
	3	3	Naphthalene	20 to 72	44
	3	2	Benz[a]anthracene	BD to 3.3	2.1
	3	3	Pyrene	48 to 100	72
	3	1	Dibenzofuran	BD to 16	16
	3	1	Diphenylamine	BD to 6.7	6.7

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

Table 4.2.32b Explosive D, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ²) ^c	Geometric Mean ^d (ng/m ²)
	Total	AD ^a			
150-m circle	3	3	2,4-Dinitrotoluene	58 to 100	80
	3	3	2,6-Dinitrotoluene	6 to 17	10
	3	3	2,4,6-Trinitrotoluene	2.7 to 130	20
	3	3	2-Nitronaphthalene	3.5 to 16	6.8
	3	3	N-Nitrosodiphenylamine	4.8 to 43	8.9
	3	3	1,3,5-Trinitrobenzene	1.5 to 28	6.9
	3	3	2-Nitrodiphenylamine	6.8 to 22	10.9
	3	3	1-Nitropyrene	2.3 to 27	7.6
	3	1	Picric acid	BD ^e to 32	32
	3	2	Naphthalene	BD to 50	22
	3	2	Benz[a]anthracene	BD to 11	2.4
	3	1	Benzo[a]pyrene	BD to 3.0	3.0
	3	2	Pyrene	BD to 16	16
	3	3	Dibenzofuran	16 to 32	23
	3	3	Diphenylamine	4.2 to 50	15
200-m circle	3	3	2,4-Dinitrotoluene	20 to 85	48
	3	3	2,6-Dinitrotoluene	6.2 to 11	8.6
	3	3	2,4,6-Trinitrotoluene	15 to 85	28
	3	3	2-Nitronaphthalene	6.7 to 13	9.4
	3	3	1,3,5-Trinitrobenzene	6.5 to 8.2	7.1
	3	3	2-Nitrodiphenylamine	7.5 to 12	9.0
	3	3	1-Nitropyrene	2.5 to 6.3	4.2
	3	2	Picric acid	BD to 37	9.2
	3	3	Naphthalene	12.2 to 47	28
	3	1	Benz[a]anthracene	BD to 3.7	3.7
	3	1	Benzo[a]pyrene	BD to 9.8	9.8
	3	3	Pyrene	5.8 to 25	13
	3	3	Dibenzofuran	8.8 to 35	16
	3	3	Diphenylamine	BD to 27	13

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

4.2.4 RDX Test - Phase C

4.2.4.1 Air Emissions

4.2.4.1.1 Gases

a. The gas EFs for the six *surface* RDX detonations are statistically summarized in Table 4.2.33. The CO₂ EF average was 0.57 for these approximate 907 kg RDX *surface* detonations. Assuming that all carbon in the explosive is converted to CO₂, the resulting theoretical EF is 0.59. The detonation efficiency, (the ratio of the measured CO₂ EF to the theoretical value) for this explosive is about 0.97. The detonation efficiency for RDX is higher (indicating a greater percentage of carbon converted to CO₂) than the detonation efficiency measured for *surface* detonated TNT, composition B, and explosive D. The fact that the RDX molecule has a higher oxygen content (-21.6 % oxygen balance) compared to TNT (-73.9 % oxygen balance), composition B (-53.0% oxygen balance), explosive D (-52.0 % oxygen balance) could be a contributing factor to the increased detonation efficiency. From this observation, it appears that the oxygen content of the explosive molecule may have an impact on the observed detonation efficiency. The relatively high and invariant carbon to CO₂ conversion efficiencies observed for these *surface* detonations also indicate the presence of a so-called "secondary combustion" mechanism, whereby ambient oxygen is entrained into the detonation fireball providing oxidant for further combustion of such incomplete detonation products as CO to CO₂.

Table 4.2.33 Gas Emission Factors for RDX Surface Detonations.

Species	Emission Factor (g/g)
CO ₂ - min	0.55
CO ₂ - max	0.58
CO ₂ - avg	0.57
CO - min	0.026
CO - max	0.039
CO - avg	0.031
NO - min	0.5×10^{-3}
NO - max	1.6×10^{-3}
NO - avg	0.9×10^{-3}
NO ₂ - min	0.4×10^{-3}
NO ₂ - max	0.9×10^{-3}
NO ₂ - avg	0.6×10^{-3}

b. The CO EFs for RDX ranged from 0.026 to 0.039, with an average of 0.031. Nitric oxide and NO₂ EFs for RDX are in the 10⁻³ range, with a ratio of about one. These values for both CO and NO_x species are comparable to those measured for surface detonated TNT.

4.2.4.1.2 Particulate Emissions

Particulate mass concentration as measured in multiple passes through the clouds from surface detonated RDX is summarized in Table 4.2.34. Cloud particle concentrations for the two three-shot tests are in the vicinity of 200 mg/m³ and are similar to those measured in the *surface* TNT, composition B, and explosive D tests. The collected particulate samples for organic and elemental carbon content were not analyzed since the Teflon[®]-coated glass fiber filters employed during the Phase C testing phase are not well suited for this analysis procedure.

Table 4.2.34 Average Particulate Concentrations Measured During Multiple Aircraft Sampling Passes of RDX Detonation Clouds.

Test Event	Particulate Matter Concentration (mg/m ³)
RDX - first 3-detonation series	242
RDX - second 3-detonation series	179

4.2.4.1.3 VOC Emissions

Volatile organic compound EFs for the RDX *surface* detonations as measured with the 6-L grab canisters and gas chromatographic analysis are summarized in Table 4.2.35. Methane emissions are low and in the range observed for the other propellants and explosives tested. Total non-methane hydrocarbon concentrations are similarly low, with an average EF of 0.0013. The toxic sub-category of TNMHC as represented by benzene is also low with an average benzene EF of 0.000069. Although detonation efficiencies less than unity are observed for this explosive, these data reveal that only a very small amount of the original carbon ends up in the VOC category of emissions.

Table 4.2.35 Volatile Organic Compound Emission Factors Measured for the RDX Detonation Tests.

Species	Emission Factor (g/g) RDX
CH ₄ - min	BD ^a
CH ₄ - max	0.4 x 10 ⁻³
CH ₄ - avg	0.2 x 10 ⁻³
TNMHC - min	0.7 x 10 ⁻³
TNMHC - max	2.9 x 10 ⁻³
TNMHC - avg	1.3 x 10 ⁻³
Benzene - min	2.3 x 10 ⁻⁶
Benzene - max	140 x 10 ⁻⁶
Benzene - avg	69 x 10 ⁻⁶

^aBelow detection limit.

4.2.4.1.4 Semivolatile Organics (Exotics)

a. Emission factors for the semivolatile organic target compounds are given in Table 4.2.36 for the Phase C RDX surface detonations. The values shown in the table are the maximum values obtained from two separate trials each consisting of three detonations in series. Analyses for the semivolatile target analytes were done by SFC-MS which allows the determination of thermally labile compounds such as the parent explosive RDX which would otherwise decompose during separation by conventional gas chromatography. The EFs for the target analytes are all observed at the part per million (10^{-6}) level or less. The highest EFs observed were for the RDX and dibenzofuran at about 2×10^{-6} . Next highest were 2,4-dinitrotoluene, naphthalene, pyrene, and diphenylamine at about 2×10^{-7} . It is not clear from these data whether the measured 2,4-dinitrotoluene and diphenylamine are derived from rearrangement of some small fraction of the RDX molecule during the detonation or whether they arise from previous contamination of the soils in the area of the surface RDX shots. One detonation of the three RDX detonations was primed with 1.8 kg of TNT (Table 2.4b) which could have been a contributor to some of these unexpected compounds; however, this alone does not explain these compounds being found when TNT was not used as a primer. It is more reasonable to attribute these compounds to the contaminated soil at the detonation site. The remainder of the target analytes were either not detected or observed at lower levels. To place these EFs into perspective consider that 1 gram of RDX parent compound would be released into the detonation cloud following the detonation of a metric ton of RDX, assuming that RDX EF is 1×10^{-6} . If a stable detonation cloud volume of 10^6 cubic meters is assumed, the elevated cloud concentration of RDX would be $1 \mu\text{g}$ per cubic meter. A further dilution of about 4 or 5 orders of magnitude would typically result following downwind movement of the cloud prior to its ground contact. Downwind ground-level concentrations of RDX would then be in the tens or hundreds of pg (10^{-12} g) per cubic meter of air.

Table 4.2.36 Maximum Semivolatile Organic Emission Factors Measured for Surface RDX Detonations^a.

Species ^b	Emission Factor (g/g)
2,4-Dinitrotoluene	210 x 10 ⁻⁹
2,6-Dinitrotoluene	41 x 10 ⁻⁹
2,4,6-Trinitrotoluene	98 x 10 ⁻⁹
2-Nitronaphthalene	49 x 10 ⁻⁹
N-Nitrosodiphenylamine	BD ^c
1,3,5-Trinitrobenzene	44 x 10 ⁻⁹
2-Nitrodiphenylamine	34 x 10 ⁻⁹
1-Nitropyrene	50 x 10 ⁻⁹
RDX	2100 x 10 ⁻⁹
Naphthalene	200 x 10 ⁻⁹
Benz[a]anthracene	93 x 10 ⁻⁹
Benzo[a]pyrene	140 x 10 ⁻⁹
Pyrene	220 x 10 ⁻⁹
Phenol	--- ^d
Dibenzofuran	2000 x 10 ⁻⁹
Diphenylamine	310 x 10 ⁻⁹

^aEmission factors are expressed in terms of 10⁻⁹ for ease of comparison, e.g., 210 x 10⁻⁹ is equivalent to 0.000000210.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels.

^cBelow detection limit.

^d---Phenol was lost in the extraction of the semivolatiles.

4.2.4.2 Soil

4.2.4.2.1 Ejecta

a. Ejecta soil is the soil displaced at the point of a *surface* detonation and redeposited in the crater, in the berm around the crater, and within a few meters of the crater. The volume of the displaced soil was estimated using Equation 4.2 paragraph, 4.1.3.3. The calculated results are given in Table 4.2.37. The volume of the displaced soil varied from 21 to 37 m³. The calculated weight of this soil, based on a density of 2.5 g/cc, varied from 52 to 94 metric tons with a mean of 67 metric tons. This loose soil was sampled, and the semivolatile organics remaining after the detonation were identified and quantified.

Table 4.2.37 OB/OD Detonation Crater Dimension, Volume, and Weight of Displaced Soil for RDX.

Location	Rim Opening (m)	Depth (m)	Volume (m ³)	Weight of Soil (kg)	Average Weight (kg)
RDX Explosive					
D1	6.5	1.5	26.65	66636	67135
D2	6.5	1.2	20.81	52037	
D3	6.0	1.5	22.97	57432	
D4	6.5	1.5	26.65	66636	
D5	7.5	2.0	37.37	93430	
D6	6.5	1.5	26.65	66636	

b. Background samples were taken at all detonation sites. All detonation sites were located in an area considered uncontaminated from previous explosive detonations. The pretest (background) and ejecta summary data are presented in Table 4.2.38. The analytes which showed increased concentrations (above concentration levels in the pretest soil) in the ejecta soil after detonation were naphthalene, pyrene, and dibenzofuran. N-nitrosodiphenylamine was found in all of the ejecta samples but not found in the soil background samples.

Table 4.2.38 RDX, Summary of Semivolatile Organic Concentrations from Phase C Pretest and Ejecta Soil Samples, Based on the Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^a			
Pretest	3	3	2,4-Dinitrotoluene	0.56 to 0.73	0.62
	3	3	2,6-Dinitrotoluene	0.056 to 0.32	0.15
	3	3	2,4,6-Trinitrotoluene	0.16 to 0.64	0.39
	3	3	2-Nitronaphthalene	0.18 to 0.51	0.31
	3	3	1,3,5-Trinitrobenzene	0.14 to 0.30	0.20
	3	3	2-Nitrodiphenylamine	0.12 to 0.30	0.19
	3	3	1-Nitropyrene	0.20 to 0.80	0.42
	3	3	RDX	1.1 to 3.8	2.3
	3	3	Naphthalene	0.11 to 0.46	0.25
	3	3	Benz[a]anthracene	0.17 to 0.18	0.18
	3	3	Benzo[a]pyrene	0.14 to 0.16	0.15
	3	3	Pyrene	0.0027 to 0.062	0.018
	3	2	Dibenzofuran	BD ^e to 0.080	0.062
	3	3	Diphenylamine	0.24 to 0.25	0.25
Ejecta	3	3	2,4-Dinitrotoluene	0.34 to 2.0	0.86
	3	3	2,6-Dinitrotoluene	0.080 to 0.90	0.27
	3	3	2,4,6-Trinitrotoluene	0.28 to 0.67	0.37
	3	3	2-Nitronaphthalene	0.13 to 0.90	0.33
	3	3	N-Nitrosodiphenylamine	0.60 to 1.7	1.2
	3	3	1,3,5-Trinitrobenzene	0.13 to 0.77	0.27
	3	3	2-Nitrodiphenylamine	0.14 to 0.19	0.17
	3	2	1-Nitropyrene	BD to 0.23	0.10
	3	3	RDX	4.9 to 15	9.6
	3	3	Naphthalene	3.1 to 5.3	4.4
	3	3	Benz[a]anthracene	1.8 to 2.4	2.1
	3	2	Benzo[a]pyrene	BD to 0.41	0.33
	3	3	Pyrene	0.53 to 5.3	2.1
	3	3	Dibenzofuran	0.69 to 0.95	0.83
	3	2	Diphenylamine	BD to 0.48	0.46

^aAbove detection limit.

^bSee Table 3.16 for list containing the semivolatile organics and the detection levels in soil.

^c μg of analyte per kg of soil.

^dGeometric means were computed only from the values above the detection limit.

^eBelow detection limit.

4.2.4.2.2 Fallout

a. Fallout for the OB/OD thermal treatment testing is defined as the particulate material deposited beyond the ejecta area. The Phase C testing was to characterize the resulting soil fallout pattern and the amount of species deposited on the soil. The background and ejecta data were included along with the fallout data, prior to performing the ANOVA.

b. In Phase C, fallout sampling for a *surface* detonation was done with 1-m² pans placed on the 50-, 100-, 150-, and 200-meter circles.

(1) The analyte concentration data from the 50- and 100-meter sampling circles for the *surface* detonations are summarized in Table 4.2.39a. The analyte concentration data for the 150- and 200-meter sampling circles are given in Table 4.2.39b. The analytes detected above background concentration levels at the 50-meter distance from detonation were RDX, benz[a]anthracene, pyrene, and diphenylamine. At the 100-meter distance RDX, dibenzofuran, and diphenylamine were detected above background concentration levels. The analytes detected above background levels at the 150-meter distance were 2,4-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 2-nitrodiphenylamine, 1-nitropyrene, RDX, naphthalene, benz[a]anthracene, benzo[a]pyrene, pyrene, dibenzofuran, and diphenylamine. The analytes detected above background levels at the 200-meter distance were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, 1-nitropyrene, RDX, naphthalene, benz[a]anthracene, benzo[a]pyrene, pyrene, dibenzofuran, and diphenylamine. N-nitrosodiphenylamine was not found in the background soil samples; however, it was found in the ejecta and fallout pan samples.

Table 4.2.39a RDX, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^e			
50-m circle	3	3	2,4-Dinitrotoluene	0.30 to 2.0	0.81
	3	3	2,6-Dinitrotoluene	0.081 to 0.84	0.26
	3	3	2,4,6-Trinitrotoluene	0.95 to 5.0	1.9
	3	3	2-Nitronaphthalene	0.36 to 1.6	0.68
	3	2	N-Nitrosodiphenylamine	BD ^e to 3.8	2.0
	3	3	1,3,5-Trinitrobenzene	0.093 to 0.92	0.23
	3	3	2-Nitrodiphenylamine	0.56 to 0.70	0.63
	3	3	1-Nitropyrene	0.045 to 1.0	0.17
	3	3	RDX	11 to 45	25
	3	3	Naphthalene	1.1 to 1.4	1.2
	3	3	Benz[a]anthracene	1.8 to 12	6.0
	3	2	Benzo[a]pyrene	BD to 2.9	2.4
	3	3	Pyrene	2.7 to 5.3	3.9
	3	1	Dibenzofuran	BD to 0.35	0.35
	3	1	Diphenylamine	BD to 0.67	0.67
100-m circle	3	3	2,4-Dinitrotoluene	0.16 to 0.79	0.39
	3	3	2,6-Dinitrotoluene	0.015 to 0.68	0.16
	3	3	2,4,6-Trinitrotoluene	0.48 to 4.8	2.1
	3	3	2-Nitronaphthalene	0.33 to 1.1	0.63
	3	2	N-Nitrosodiphenylamine	BD to 4.2	0.38
	3	3	1,3,5-Trinitrobenzene	0.0075 to 0.28	0.081
	3	3	2-Nitrodiphenylamine	0.051 to 1.2	0.75
	3	2	1-Nitropyrene	BD to 1.5	0.70
	3	3	RDX	8.6 to 130	32
	3	3	Naphthalene	0.82 to 1.8	1.1
	3	2	Benz[a]anthracene	BD to 8.8	1.3
	3	3	Benzo[a]pyrene	0.022 to 0.98	0.22
	3	3	Pyrene	0.0038 to 5.7	0.38
	3	1	Dibenzofuran	BD to 3.1	3.1

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

Table 4.2.39b RDX, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Weight of Sample.

Source of Sample	Number of Observations		Analyte ^b	Range Response ($\mu\text{g}/\text{kg}$) ^c	Geometric Mean ^d ($\mu\text{g}/\text{kg}$)
	Total	AD ^a			
150-m circle	3	3	2,4-Dinitrotoluene	2.2 to 110	21
	3	3	2,6-Dinitrotoluene	0.82 to 130	5.5
	3	3	2,4,6-Trinitrotoluene	12 to 150	62
	3	2	2-Nitronaphthalene	BD ^e to 120	21
	3	3	N-Nitrosodiphenylamine	6.6 to 210	30
	3	3	1,3,5-Trinitrobenzene	0.79 to 200	5.5
	3	2	2-Nitrodiphenylamine	BD to 78	20
	3	2	1-Nitropyrene	BD to 120	26
	3	2	RDX	BD to 1400	1000
	3	3	Naphthalene	15 to 210	47
	3	2	Benz[a]anthracene	BD to 220	19
	3	3	Benzo[a]pyrene	2.5 to 160	11
	3	3	Pyrene	9.0 to 250	30
	3	2	Dibenzofuran	BD to 93	32
	3	1	Diphenylamine	BD to 86	86
200-m circle	3	3	2,4-Dinitrotoluene	16 to 260	73
	3	2	2,6-Dinitrotoluene	BD to 66	16
	3	3	2,4,6-Trinitrotoluene	6.5 to 150	27
	3	3	2-Nitronaphthalene	6.5 to 150	27
	3	3	N-Nitrosodiphenylamine	15 to 170	40
	3	3	1,3,5-Trinitrobenzene	5.9 to 95	16
	3	3	2-Nitrodiphenylamine	4.9 to 35	17
	3	3	1-Nitropyrene	7.8 to 71	18
	3	3	RDX	290 to 1100	680
	3	3	Naphthalene	9.5 to 740	66
	3	3	Benz[a]anthracene	30 to 60	40
	3	1	Benzo[a]pyrene	BD to 79	79
	3	3	Pyrene	35 to 230	69
	3	2	Dibenzofuran	BD to 46	40
	3	3	Diphenylamine	18 to 46	28

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents μg of analyte per kg of soil.

^dGeometric means were computed from the values above the detection limit.

^eBelow detection limit.

(2) The Duncan's multiple-range test comparing the ejecta sample results with the fallout sample results for the semivolatile organics shows the following:

(a) The 50-meter concentration means were not different than the ejecta concentration means.

(b) The 100-meter analyte concentration means were not different from the ejecta concentration means.

(c) The analytes detected above ejecta concentration levels at the 150-meter distance were 2,4-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 2-nitrodiphenylamine, 1-nitropyrene, RDX, naphthalene, dibenzofuran, and diphenylamine.

(d) The analytes detected above ejecta concentration levels at the 200-meter distance were 2,4-dinitrotoluene, 2,6-dinitrotoluene, 2,4,6-trinitrotoluene, 2-nitronaphthalene, 1,3,5-trinitrobenzene, 2-nitrodiphenylamine, 1-nitropyrene, RDX, naphthalene, benz[a]pyrene, dibenzofuran, and diphenylamine.

(3) This increase in concentration of the semivolatile analytes on the fallout soil at greater distance from the detonation may be a function of particle size (the increased surface area per volume of particle that results with the smaller particles provides more surface area for absorption of the analyte.) The results of OB/OD test show that analytes in the 200-, 150, and 100-meter fallout samples were more concentrated than in the 50-meter fallout samples. The results did not show the 50-meter analyte concentrations to be greater than the ejecta concentration means. A probable explanation of the increased concentration of analytes with distance is that soil chunks are still being propelled as far as 50 meter and the sample is a composite of a wide range of particle sizes including the larger chunks whose interior volume is not exposed to detonation products. This is in contrast to the fallout samples at greater distances, which consist of smaller particles.

(4) The mass of analyte collected was compared to the total sampling area of the fallout pans comprising the sample. Those data are summarized in Tables 4.2.40a and 4.2.40b. These data are useful in estimating the amount of an analyte that is deposited on the terrain as a function of distance from the source.

Table 4.2.40a RDX, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ²) ^c	Geometric Mean ^d (ng/m ²)
	Total	AD ^a			
50-m circle	3	3	2,4-Dinitrotoluene	27 to 170	69
	3	3	2,6-Dinitrotoluene	6.6 to 69	22
	3	3	2,4,6-Trinitrotoluene	78 to 450	160
	3	3	2-Nitronaphthalene	30 to 130	58
	3	2	N-Nitrosodiphenylamine	BD ^e to 310	160
	3	3	1,3,5-Trinitrobenzene	7.5 to 76	20
	3	3	2-Nitrodiphenylamine	50 to 57	53
	3	3	1-Nitropyrene	3.7 to 83	14
	3	3	RDX	890 to 4100	2100
	3	3	Naphthalene	95 to 120	110
	3	3	Benz[a]anthracene	150 to 960	500
	3	2	Benzo[a]pyrene	BD to 260	200
	3	3	Pyrene	220 to 430	330
	3	1	Dibenzofuran	BD to 29	29
	3	1	Diphenylamine	BD to 55	55
100-m circle	3	3	2,4-Dinitrotoluene	7.2 to 18	12
	3	3	2,6-Dinitrotoluene	0.67 to 15	4.8
	3	3	2,4,6-Trinitrotoluene	22 to 170	67
	3	3	2-Nitronaphthalene	13 to 28	19
	3	2	N-Nitrosodiphenylamine	BD to 72	10
	3	3	1,3,5-Trinitrobenzene	0.33 to 11	2.5
	3	3	2-Nitrodiphenylamine	3.2 to 20	11
	3	2	1-Nitropyrene	BD to 25	18
	3	3	RDX	380 to 2200	980
	3	3	Naphthalene	30 to 37	34
	3	2	Benz[a]anthracene	BD to 150	35
	3	3	Benzo[a]pyrene	1.0 to 20	6.9
	3	3	Pyrene	0.17 to 100	12
	3	1	Dibenzofuran	BD to 53	53

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cRepresents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

Table 4.2.40b RDX, Summary of Semivolatile Organic Concentrations from Phase C Fallout Soil Samples, Based on Area Sampled.

Source of Sample	Number of Observations		Analyte ^b	Range Response (ng/m ²) ^c	Geometric Mean ^d (ng/m ²)
	Total	AD ^a			
150-m circle	3	3	2,4-Dinitrotoluene	8.2 to 83	32
	3	3	2,6-Dinitrotoluene	1.8 to 57	8.4
	3	3	2,4,6-Trinitrotoluene	47 to 280	95
	3	2	2-Nitronaphthalene	BD ^e to 50	27
	3	3	N-Nitrosodiphenylamine	15 to 92	46
	3	3	1,3,5-Trinitrobenzene	2.3 to 85	8.4
	3	2	2-Nitrodiphenylamine	BD to 33	26
	3	2	1-Nitropyrene	BD to 52	33
	3	2	RDX	BD to 2700	1300
	3	3	Naphthalene	33 to 120	72
	3	2	Benz[a]anthracene	BD to 93	24
	3	3	Benzo[a]pyrene	5.7 to 70	17
	3	3	Pyrene	20 to 110	46
	3	2	Dibenzofuran	BD to 40	32
	3	1	Diphenylamine	BD to 37	37
200-m circle	3	3	2,4-Dinitrotoluene	38 to 68	49
	3	2	2,6-Dinitrotoluene	BD to 27	21
	3	3	2,4,6-Trinitrotoluene	3.3 to 38	15
	3	3	2-Nitronaphthalene	3.7 to 58	18
	3	3	N-Nitrosodiphenylamine	5.8 to 120	27
	3	3	1,3,5-Trinitrobenzene	1.0 to 38	11
	3	3	2-Nitrodiphenylamine	4.8 to 22	11
	3	3	1-Nitropyrene	1.3 to 50	12
	3	3	RDX	120 to 4800	450
	3	3	Naphthalene	17 to 130	44
	3	3	Benz[a]anthracene	10 to 130	27
	3	1	Benzo[a]pyrene	BD to 32	32
	3	3	Pyrene	17 to 150	46
	3	2	Dibenzofuran	BD to 18	10
	3	3	Diphenylamine	4.3 to 80	19

^aAbove detection limit.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels in soil.

^cP represents ng of analyte per m² of terrain.

^dGeometric means were computed from the values above detection limit.

^eBelow detection limit.

4.3 Propellants

4.3.1 Single Base Tests - Phase C

4.3.1.1 M-1 Propellant

4.3.1.1.1 Air Emissions

a. Gases

(1) Gas EFs for the M-1 single base propellant burns during the Phase C test series are given in Table 4.3.1. Measured CO₂ EFs for M-1 were the same for all test burns at a value of 1.11. Assuming that all the carbon in the original propellant is converted to CO₂, the resulting theoretical EF is also 1.11 when calculated to two decimal places. The equivalence of the measured and theoretical EFs (to two decimal places) reveals that greater than 99-percent conversion of propellant carbon to CO₂ is occurring in these large-scale burns.

Table 4.3.1 Gas and VOC Emission Factors for M-1 Single Base Propellant.

Species	Emission Factor (g/g)
CO ₂ - min	1.11
CO ₂ - max	1.11
CO ₂ - avg	1.11
Number of observations	6
CO - min	5.4×10^{-6}
CO - max	900×10^{-6}
CO - avg	250×10^{-6}
Number of observations	4
NO - min	760×10^{-6}
NO - max	1600×10^{-6}
NO - avg	1200×10^{-6}
Number of observations	6
NO ₂ - min	410×10^{-6}
NO ₂ - max	510×10^{-6}
NO ₂ - avg	470×10^{-6}
Number of observations	6
CH ₄ - min	BD ^a
CH ₄ - max	49000×10^{-6}
CH ₄ - avg	8000×10^{-6}
Number of observations	8
TNMHC - min	BD
TNMHC - max	2000×10^{-6}
TNMHC - avg	460×10^{-6}
Number of observations	8
Benzene - min	BD
Benzene - max	25×10^{-6}
Benzene - avg	4.8×10^{-6}
Number of observations	8

^aBelow detection limit.

(2) Carbon monoxide EFs for M-1 are very low and in the 10^{-4} to 10^{-5} range. This is not surprising, considering the high CO_2 EFs encountered. Nitric oxide EFs for M-1 are in the range of 1×10^{-3} and are similar to those encountered for the *surface* TNT tests. Nitrogen dioxide levels are about a factor of ten lower, although as noted in an earlier section on total NO_x emission from TNT tests, it can be conservatively estimated that all NO produced in the burn will eventually be converted to NO_2 . Correcting this assumption for the mass difference between the NO and the NO_2 molecule results in an average NO_2 EF for M-1 of 0.0023.

b. Particulate Matter

(1) Mass concentrations within the cloud during the Phase C September 5 and 6 M-1 tests were in the range of 1.3 to 2.6 mg m^{-3} as averaged over three passes in a time interval of about 4 minutes following propellant ignition. If the assumption is made that all particulate in the cloud is derived from the propellant and none is entrained soil, these measured cloud concentrations translate to a range of total particulate EFs between 4.5×10^{-3} and 9.2×10^{-3} , or between 0.5 and 1 percent of the propellant. Data from the wing-mounted aerosol probes reveals that the sizes of particles encountered in the cloud are all within the range that can be efficiently sampled by the aircraft inlet probe and transport tube. As a result the collected particulate mass can be reasonably interpreted as a total particulate mass.

c. Volatile Organic Compounds

(1) Emission factors for representative VOC's for the M-1 are given in Table 4.3.1. Considering the high carbon conversion efficiencies noted for both of these propellant types, it is not surprising that EFs for methane, TNMHC, and benzene appear at low levels. Methane shows the most variability with EFs ranging from the 10^{-2} level down to a non-detectable level. TNMHC levels range from the 10^{-4} level to non-detectable levels and are similar to those measured in TNT tests. Consistent with observations in the TNT tests, the TNMHC category is principally composed of non-toxic light weight gases such as ethane, propane, acetylene, etc. Benzene is observed at low concentration levels of about 5 $\mu\text{g/g}$ of the M-1 propellant burned.

d. Semivolatile Organics

(1) Emission factors for the semivolatile organic category for the M-1 tests are given in Table 4.3.2. As a conservative estimate, only the maximum value determined in two discrete measurements is given in the table. As was noted for the TNT tests, most of the target analytes were below the detection level of the analytical instrument. Species observed above the detection level for the M-1 propellant include 2,4-DNT, phenol, naphthalene, and diphenylamine. Of all target analytes, naphthalene was detected at the highest concentration. This level corresponds to an EF of about 2×10^{-9} , which is still quite low in the context of air emissions.

Table 4.3.2 Semivolatile Organic Emission Factors for M-1 Single Base Propellant.

Species	Emission Factor (g/g)
2,4-Dinitrotoluene	1.2×10^{-9}
2,6-Dinitrotoluene	BD*
2,4,6-Trinitrotoluene	BD
2-Nitronaphthalene	BD
N-Nitrosodiphenylamine	BD
1,3,5-Trinitrobenzene	BD
1-Nitropyrene	BD
Naphthalene	19×10^{-9}
Benz[a]anthracene	BD
Benzo[a]pyrene	BD
Pyrene	BD
Phenol	3.4×10^{-9}
Dibenzofuran	BD
Diphenylamine	0.11×10^{-9}

*Below detection limit, which is less than 10×10^{-9} for most of the target analytes.

4.3.1.1.2 Soil Deposition

a. Sputter

Ten sputter pan samples were placed 1 meter from the burn pans to collect propellant granules ejected from the burn pans during the burn. All M-1 propellant residue landing in the powdery soil or collected in the 1-m² pans visually appeared to be charred residue. This observation was substantiated by the low level of the analytes recovered. The mass of ash collected in the sputter

pans averaged 8.76 g/m² on trial 1 and 5.61 g/m² on trial 2. The concentration of each analyte expressed as ng/g and ng/m² of soil surface are given in Table 4.3.3.

Table 4.3.3 Summary of Semivolatile Organic Concentrations from M-1 Propellant Burn, Sputter Pan Sampling.

Analyte	Number of Observations		Concentration Range	
	Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	2	2	81 to 160	440 to 850
2,6-Dinitrotoluene	2	2	1.4 to 4.1	7.8 to 22
2,4,6-Trinitrotoluene	2	1	BD ^d to 0.11	BD to 0.57
2-Nitronaphthalene	2	1	BD to 0.14	BD to 0.73
2-Nitrodiphenylamine	2	2	0.22 to 0.29	1.2 to 1.5
Naphthalene	2	2	1.4 to 5.5	7.3 to 30
Benz[a]anthracene	2	1	BD to 0.15	BD to 0.81
Diphenylamine	2	2	3.7 to 6.9	20 to 37

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

b. Fallout

Fallout pan samplers were placed in concentric circles 6 and 12 meters from the center of the burn pan array. The mass of ash collected in the pans at 6 meters was 7.5 and 2.2 g/m² on trial 1 and trial 2, respectively. The mass of ash collected in the pans at 12 meters was 0.88 and 0.61 g/m² for trial 1 and trial 2, respectively. No sampling was done beyond 12 meters on the M-1 burns; however, sampling beyond this distance on previous burns resulted in insufficient fallout for quantification of any of the analytes of interest. The analyte concentration data from the 6- and 12-meter fallout pans are summarized in Table 4.3.4. Using the maximum measured 2,4-dinitrotoluene concentration of 2800 ng/m² as representative of the terrain deposition out to 18 meters, results in a total deposition of 2.87 mg of 2,4-DNT spread over the 1000 m² or 0.25 acre.

Table 4.3.4 Summary of Semi-volatile Analyte Concentrations from M-1 Propellant Burn, Fallout Pan Sampling.

Analyte	Sample Distance (m)	Number of Observations		Concentration Range	
		Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	6	2	2	310 to 510	970 to 1800
	12	2	2	530 to 900	1100 to 2800
2,6-Dinitrotoluene	6	2	2	12 to 12	36 to 37
	12	2	2	8.9 to 36	19 to 110
2,4,6-Trinitrotoluene	6	2	2	0.12 to 0.22	0.38 to 0.69
	12	2	1	BD ^d to 0.38	BD to 0.79
2-Nitronaphthalene	6	2	2	0.094 to 0.14	0.29 to 0.44
	12	2	0	BD	BD
2-Nitrodiphenylamine	6	2	1	BD to 0.14	BD to 0.44
	12	2	0	BD	BD
Naphthalene	6	2	1	BD to 0.017	BD to 0.052
	12	2	1	BD to 2.6	BD to 8.2
Benz[a]anthracene	6	2	2	0.13 to 0.16	0.40 to 0.51
	12	2	1	BD to 0.51	BD to 1.1
Diphenylamine	6	2	2	0.51 to 0.79	1.6 to 2.5
	12	2	2	0.49 to 2.2	1.5 to 4.6

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

c. Burn Pan Residue

Burn pan residue for each 3160 kg of M-1 propellant burned varied from 3.4 kg to 4.6 kg over the six burns. The average residual was 4.0 kg or about 0.1 percent of the initial weight of propellant. Burn pan residue samples for semivolatile organic analyses were taken on each burn. A composite sample for each of the two M-1 burn trials was analyzed. The semivolatile organic analytes detected and the concentrations are given in Table 4.3.5. The residue consisted primarily of elemental and inorganic carbon. Approximately 27 µg of semivolatile organic compounds were recovered from each gram of burn pan residue. The mass fraction of 2,4-DNT in the original propellant is 0.10. After burning, the mass fraction of 2,4-DNT in the residue is 0.000025. The marked reduction of

2,4-DNT in the propellant residue is consistent with the observation that the bulk of the residue is char or elemental carbon.

Table 4.3.5 Summary of Semivolatile Analyte Concentrations from M-1 Propellant Burn, Burn Pan Residue.

Analyte	Number of Observations		Concentration Range (ng/g) ^b
	Total	AD ^a	
2,4-Dinitrotoluene	2	2	13000 to 25000
2,6-Dinitrotoluene	2	2	610 to 1200
2,4,6-Trinitrotoluene	2	2	3.7 to 15
2-Nitronaphthalene	2	2	6.1 to 6.9
N-Nitrosodiphenylamine	2	2	16 to 110
2-Nitrodiphenylamine	2	1	BD ^c to 23
Naphthalene	2	2	5.2 to 16
Benz[a]anthracene	2	2	0.63 to 4.0
Diphenylamine	2	2	56 to 180

^aAbove detection limit.

^bRepresents ng of analyte per gram of pan residue.

^cBelow detection limit.

4.3.1.1.3 Total Release of 2,4-Dinitrotoluene

Based on the analysis results for M-1, estimates of total release of a typical target analyte such as 2,4-DNT can be estimated as follows. The original weight fraction of 2,4-DNT in the M-1 parent compound is about 0.10 (see Table 3.4). Based on fallout pan analysis, total release to the soil surrounding the burn pan is about 3 mg. Based on residue analysis, an estimate of the total amount of 2,4-DNT in the burn residue is about 100 mg. Based on the measured emission air factor, the total release of 2,4-DNT to the air is also about 3 mg. The total release of DNT to all receptors is therefore in the order of 100 mg. The amount of 2,4-DNT in the original weight of M-1 prior to ignition is about 300 kg. Using these estimates, the mass fraction of 2,4 DNT not consumed in the burn is about 0.0000003. In other words, all but about 0.3 ppm of the original 2,4-DNT is consumed in the combustion process and oxidized to CO₂.

4.3.1.2 M-6 Propellant

4.3.1.2.1 Air Emissions

a. Gases

(1) Gas EFs for the M-6 single base propellant burns during the Phase C test series are given in Table 4.3.6. Measured CO₂ EFs for M-6 were the same for all test burns at a value of 1.06. Assuming that all the carbon in the parent material is converted to CO₂, the resulting theoretical EF is also 1.06 when calculated to two decimal places. The equivalence of the measured and theoretical EFs (to two decimal places) reveals that greater than 99-percent conversion of propellant carbon to CO₂ is occurring in these large-scale burns.

Table 4.3.6 Gas and VOC Emission Factors for the M-6 Single Base Propellant.

Species	Emission Factor (g/g)
CO ₂ - min	1.06
CO ₂ - max	1.06
CO ₂ - avg	1.06
Number of observations	6
CO - min	BD ^a
CO - max	470 x 10 ⁻⁶
CO - avg	95 x 10 ⁻⁶
Number of observations	9
NO - min	2300 x 10 ⁻⁶
NO - max	2600 x 10 ⁻⁶
NO - avg	2400 x 10 ⁻⁶
Number of observations	6
NO ₂ - min	470 x 10 ⁻⁶
NO ₂ - max	580 x 10 ⁻⁶
NO ₂ - avg	520 x 10 ⁻⁶
Number of observations	6
CH ₄ - min	1.3 x 10 ⁻⁶
CH ₄ - max	390 x 10 ⁻⁶
CH ₄ - avg	46 x 10 ⁻⁶
Number of observations	9
TNMHC - min	BD
TNMHC - max	69 x 10 ⁻⁶
TNMHC - avg	13 x 10 ⁻⁶
Number of observations	9
Benzene - min	BD
Benzene - max	7.3 x 10 ⁻⁶
Benzene - avg	1.7 x 10 ⁻⁶
Number of observations	9

^aBelow detection limit.

(2) Carbon monoxide EFs for M-6 are very low and in the range 10^{-4} to below detection level. This is not surprising considering the very high CO_2 EFs encountered. Nitric oxide EFs for M-6 are in the range of 0.002 and are similar to those encountered for the *surface* TNT tests. Nitrogen dioxide levels are about a factor of 10 lower, although as noted in an earlier section on total NO_x emission from TNT tests, it can be conservatively estimated that all NO produced in the burn will eventually be converted to NO_2 . With this assumption and correcting for the mass difference between the NO and the NO_2 molecule, the average NO_2 EF for M-6 would be 0.0042.

b. Particulate Matter

(1) Mass concentrations within the cloud during the Phase C August 29 and 30 M-6 tests reveal cloud concentrations in the range of 2.7 to 2.8 mg/m^3 as averaged over three passes in a time interval of about 4 minutes following propellant ignition. Assuming that all particulate in the cloud is derived from the propellant and none is entrained soil, these measured cloud concentrations translate to a range of total particulate EFs between 9.0×10^{-3} to 1.2×10^{-2} , or very near 1 percent of the propellant. Data from the wing-mounted aerosol probes reveals that the sizes of particles encountered in the cloud are all within the range that can be efficiently sampled by the aircraft inlet probe and transport tube. As a result the collected particulate mass can be reasonably interpreted as a "total" particulate mass.

c. Volatile Organic Compounds

(1) Emission factors for representative VOC's for the M-6 are given in Table 4.3.6. Considering the high carbon conversion efficiencies noted for M-6 propellant, it is no surprise that EFs for methane, TNMHC and benzene appear at low levels. The average EFs for methane, TNMHC, and benzene are 0.000046, 0.000013, and 0.0000017, respectively. Like the TNT results, the TNMHC category is principally composed of non-toxic light weight gases, such as ethane, propane, acetylene, etc.

d. Semivolatile Organics

(1) Emission factors for the semivolatile organic category from the M-6 tests are given in Table 4.3.7. As a conservative estimate, only the maximum value determined in two discrete measurements for each propellant is given in the table. As was noted for the TNT tests, most of the target analytes were below the detection level of the analytical instrument. Species observed above the detection level for the M-6 propellant include 2,4-DNT, 2,6-DNT, N-nitrosodiphenylamine, phenol, naphthalene, and diphenylamine. Of all target analytes, naphthalene was detected at the highest concentration. This level corresponds to an EF of about 75×10^{-9} .

Table 4.3.7 Semivolatile Organic Emission Factors for M-6 Single Base Propellants.

Species	Emission Factor (g/g)
2,4 Dinitrotoluene	1.0×10^{-9}
2,6 Dinitrotoluene	0.077×10^{-9}
2,4,6 Trinitrotoluene	BD*
2-Nitronaphthalene	BD
N-Nitrosodiphenylamine	0.14×10^{-9}
1,3,5-Trinitrobenzene	BD
1-Nitropyrene	BD
Naphthalene	75×10^{-9}
Benz[a]anthracene	BD
Benzo[a]pyrene	BD
Pyrene	BD
Phenol	1.5×10^{-9}
Dibenzofuran	BD
Diphenylamine	0.026×10^{-9}

*Below detection limit, which is less than 10×10^{-9} for most target analytes.

4.3.1.2.2 Soil Deposition

a. Sputter

Ten sputter pan samples were placed 1 meter from the burn pans to collect propellant granules ejected from the burn pans during the burn. All M-6 propellant residue landing in the powdery soil or collected in the 1-m² pans visually appeared to be charred residue. This observation was substantiated by the low level of the analytes recovered. The mass of ash collected in the sputter

pans averaged 24.2 g/m². The concentration of each analyte expressed as ng/g and ng/m² of terrain surface are given in Table 4.3.8.

Table 4.3.8 Summary of Semivolatile Analyte Concentrations from M-6 Burn, Sputter Pan Sampling.

Analyte	Number of Observations		Concentration Range	
	Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	3	3	8.1 to 12	44 to 66
2,4,6-Trinitrotoluene	3	1	BD ^d to 0.004	BD to 0.022
2-Nitronaphthalene	3	2	BD to 0.010	BD to 0.056
1,3,5-Trinitrobenzene	3	1	BD to 0.009	BD to 0.048
1-Nitropyrene	3	1	BD to 0.009	BD to 0.049
Naphthalene	3	3	0.34 to 1.00	1.9 to 5.4
Benz[a]anthracene	3	1	BD to 0.51	BD to 2.7
Benzo[a]pyrene	3	2	BD to 0.34	BD to 1.9
Pyrene	3	1	BD to 0.30	BD to 1.6
Phenol	3	1	BD to 0.14	BD to 0.78
Dibenzofuran	3	2	BD to 1.4	BD to 7.7
Diphenylamine	3	3	0.16 to 4.0	0.88 to 22

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

b. Fallout

Fallout pan samplers were placed in concentric circles 6 and 12 meters from the center of the burn pan array. The mass of ash collected in the pans at 6 meters was 8.6 g/m². The mass of ash collected in the pans at 12 meters was 2.8 g/m². No sampling was done beyond 12 meters on the M-6 burns; however, sampling beyond this distance on other propellant burns resulted in insufficient fallout for quantification of any of the analytes of interest. The analyte concentration data from the 6- and 12-meter fallout pans are summarized in Table 4.3.9. Using the maximum measured 2,4-dinitrotoluene concentration of 1300 ng/m² as representative of the terrain deposition out to 18 meter, results in a total deposition of 1.32 mg of 2,4-DNT spread over 1000 m² or 0.25 acre.

Table 4.3.9 Summary of Semivolatile Analyte Concentrations from M-6 Burn, Fallout Pan Sampling.

Analyte	Sample Distance (m)	Number of Observations		Concentration Range	
		Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	6	3	3	45 to 410	140 to 1300
	12	3	3	37 to 230	110 to 480
2,4,6-Trinitrotoluene	6	3	1	BD ^d to 0.786	BD to 2.5
	12	3	3	0.088 to 1.0	0.28 to 3.1
2-Nitronaphthalene	6	3	2	BD to 0.11	BD to 0.34
	12	3	3	0.007 to 0.18	0.21 to 0.55
N-Nitrosodiphenylamine	6	3	1	BD to 20	BD to 63
	12	3	1	BD to 4.0	BD to 13
2-Nitrodiphenylamine	6	3	1	BD to 1.1	BD to 3.5
	12	3	1	BD to 0.16	BD to 0.49
Naphthalene	6	3	2	BD to 0.84	BD to 2.6
	12	3	2	BD to 9.6	BD to 30
Benz[a]anthracene	6	3	3	0.12 to 2.2	0.38 to 6.8
	12	3	1	BD to 0.062	BD to 0.13
Benzo[a]pyrene	6	3	3	0.18 to 1.1	0.57 to 3.5
	12	3	0	BD	BD
Pyrene	6	3	2	BD to 0.36	BD to 1.1
	12	3	0	BD	BD
Phenol	6	3	1	BD to 0.15	BD to 0.46
	12	3	0	BD	BD
Dibenzofuran	6	3	3	2.0 to 53	6.1 to 170
	12	3	2	BD to 2.8	BD to 8.9
Diphenylamine	6	3	3	0.44 to 26	1.4 to 83
	12	3	3	0.28 to 5.6	0.58 to 18

^aAbove detection limit.

^brepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

c. Burn Pan Residue

Burn pan residue for each 3200 kg of M-6 propellant burned varied from 2.3 to 3.2 kg, the average residue was 2.6 kg or about 0.1 percent of the original propellant mass. Burn pan residue samples for semivolatile analyses were taken on each burn trial, with a composite sample for each of the four M-6 burn trials analyzed. The semivolatile analytes detected and their concentrations are given in Table 4.3.10. The residue consisted primarily of elemental and inorganic carbon. Approximately 200 μ g of semivolatile organic compounds were recovered from each gram of residue. The mass fraction of 2,4-DNT in the M-6 propellant was 0.10. After burning, the mass fraction of 2,4-DNT in the residue was 0.00013. Based on these results, the semivolatile organic fraction in the propellant residue is very low, corresponding to about 0.000000103 of the original propellant weight prior to burning. The marked reduction of 2,4-DNT in the propellant residue is consistent with the observation that the bulk of the residue is char or elemental carbon.

Table 4.3.10 Summary of Semivolatile Analyte Concentrations From M-6 Burn, Burn Pan Residue.

Analyte	Number of Observations		Concentration Range (ng/g) ^b
	Total	AD ^a	
2,4-Dinitrotoluene	6	6	10000 to 130000
2,4,6-Trinitrotoluene	6	6	3.7 to 280
2-Nitronaphthalene	6	6	8.2 to 160
2-Nitrodiphenylamine	6	6	14 to 320
Naphthalene	6	2	BD ^c to 860
Benz[a]anthracene	6	5	BD to 680
Pyrene	6	4	BD to 280
Dibenzofuran	6	6	150 to 72000
Diphenylamine	6	6	62 to 2000

^aAbove detection limit.

^bRepresents ng of analyte per gram of pan residue.

^cBelow detection limit.

4.3.1.2.3 Total Release of 2,4-Dinitrotoluene

Based on the analysis results for M-6, estimates of total release of a typical target analyte such as 2,4-DNT can be estimated as follows. The original weight fraction of 2,4-DNT in the M-6 parent compound is about 0.10 (see Table 3.5). Based on fallout pan analysis, total release to the soil surrounding the burn pan is about 1.3 mg. Based on residue analysis, an estimate of the total amount of 2,4-DNT in the burn residue is about 400 mg. Based on the measured emission air factor, the total release of 2,4-DNT to the air is also about 3 mg. The total release of DNT to all receptors is therefore in the order of 400 mg. The amount of 2,4-DNT in the original weight of M-6 prior to ignition is about 300 kg. Using these estimates, the mass fraction of 2,4 DNT not consumed in the burn is about 0.0000013. In other words, all but about 1.3 ppm of the original 2,4-DNT is consumed in the combustion process and oxidized to CO_2 .

4.3.2 Triple Base Test - Phase A

4.3.2.1 Air Emissions

4.3.2.1.1 Gases

a. Gas EFs for the Triple Base Propellant burn carried out during the Phase A test series are statistically summarized in Table 4.3.11. Minimum and maximum EFs are given for important gaseous species. Sample size was limited to two samples for most species in this particular test event. The CO_2 EF was observed to be 0.66 in both samples collected. This compares with a theoretical CO_2 EF of 0.65 for this particular propellant, assuming that all propellant carbon is converted to CO_2 . This observation is accompanied by very low (~ 0.00003) EFs for CO. This trend of high carbon conversion to CO_2 is consistent with observations made on the M-1 and M-6 single-base propellants. A single measurement of NO and NO_2 which was completed on this particular test reveals an EF in the 10^{-3} range and similar to those encountered with the M-1 and M-6 propellants. Assuming total conversion of emitted NO to NO_2 , the total NO_2 EF is very near 1 percent for this propellant.

Table 4.3.11 Gas Emission Factors for Triple Base Propellants.

Species	Emission Factor (g/g)
CO ₂ - min	0.66
CO ₂ - max	0.66
CO ₂ - avg	0.66
Number of observations	2
CO - min	20×10^{-6}
CO - max	30×10^{-6}
CO - avg	25×10^{-6}
Number of observations	2
NO - min	5.2×10^{-3}
NO - max	5.2×10^{-3}
NO - avg	5.2×10^{-3}
Number of observations	1
NO ₂ - min	2.1×10^{-3}
NO ₂ - max	2.1×10^{-3}
NO ₂ - avg	2.1×10^{-3}
Number of observations	1

4.3.2.1.2 Particulate Matter

a. Precision weighing was not carried out on the filter samples from the Phase A tests. As a result, only rough estimates of particulate mass concentrations in the cloud are available. Particulate concentrations in the cloud were determined to be about 4 mg/m³ for the two-burn sequence. This cloud concentration corresponds to a particulate matter EF of about 2 percent. Some existing evidence suggests that some of the particles in the cloud were soil particles entrained in the smoke column from the burning propellant; however, further testing is required to establish this fact.

4.3.2.1.3 Volatile Organic Compounds

a. Emission factors for principal VOC compounds are given in Table 4.3.12. All species given in the table were below detection, with the exception of the TNMHC category. Levels at this

category were very low (10^{-6}). These observations are consistent with the low VOC emissions observed for the M-1 and M-6 propellant tests.

Table 4.3.12 Volatile Organic Compound Emission Factors for Triple-Base Propellant.

Species	Emission Factor (g/g)
CH ₄ - min	BD*
CH ₄ - max	BD
CH ₄ - avg	BD
Number of observations	2
TNMHC - min	0.34×10^{-6}
TNMHC - max	2.6×10^{-6}
TNMHC - avg	1.5×10^{-6}
Number of observations	2
Benzene - min	BD
Benzene - max	BD
Benzene - avg	BD
Number of observations	2

*Below detection limit.

4.3.2.1.4 Semivolatile Organic Compounds

a. All target analytes were at or below the analytical detection limit for the triple-base propellant. The detection limit for most of these semivolatile organics corresponds to a range of about 10^{-8} to 10^{-9} . These results yield further evidence of the clean burning nature of many of these propellant types.

4.3.2.2 Soil Deposition

4.3.2.2.1 Sputter

No samples were collected in close proximity to the burn pans. A visual inspection of the area after the burn showed a number of small indentations in the powdery soil. Each indentation contained a charred skeleton of the M-30 propellant granule. These indentations extended out approximately

3 meters from the burn pan. A sample of these char residues was collected and assayed by both GC-MS and SFC-MS. None of the semivolatile compounds on the analyte list were detected.

4.3.2.2.2 Fallout

A composite sample composed of fallout from the 6- and 12-meter sampling circles was assayed. The compounds detected and the concentrations were phenol, 190 $\mu\text{g/g}$; ethyl centralite, 96 $\mu\text{g/g}$; nitroglycerin, 43 $\mu\text{g/g}$; and nitroguanidine, 55 $\mu\text{g/g}$. Fallout pan samples were also placed on a circle 30 meters from the burn pans; however, the amount of fallout material collected at this range was too small for a valid chemical assay.

4.3.2.2.3 Burn Pan Residue

The analytes and the concentrations detected in the burn pan residue were phenol, 0.12 $\mu\text{g/g}$; 2-nitrodiphenylamine, 0.51 $\mu\text{g/g}$; ethyl centralite, 2.8 $\mu\text{g/g}$; nitroglycerin, 0.73 $\mu\text{g/g}$; and, nitroguanidine, 0.79 $\mu\text{g/g}$.

4.3.3 Manufacturing Residue Tests - Phases B and C

4.3.3.1 Manufacturing Residue Test - Phase B

4.3.3.1.1 The composition of the propellants in the manufacturing residue was known to contain ammonium perchlorate and some metals which would release undesirable emittant products during combustion. These emissions need to be quantified prior to RCRA Sub-part X permitting.

4.3.3.1.2 During the BB study a special task force from Battelle Columbus Division drew samples during the BB study to identify/quantify the PCDD's and PCDF's (Reference BB Volume-2, Appendix B; also BB Volume-1, paragraphs 5.7.6 and 5.7.7, page 5-22, and BB Volume-2, paragraphs 7.3.2.10 and 7.3.2.11, page 7-19)

4.3.3.1.3 Sampling for HCL during the BB study was not conclusive due to the inability of sampling to account for a chlorine balance from the composite propellant (Reference BB Volume-1, paragraph 5.7.5, page 5-22, and BB Volume-2, paragraph 7.3.2.9, pages 7-18 and 7-19).

4.3.3.1.4 During the BB study, metals were sampled successfully on Teflon™ filter media (Reference BB Volume-1, paragraph 5.7.4, page 5-17, table 5.5c, page 5-20; and BB Volume-2, paragraph 7.3.2.6, page 7-18).

4.3.3.1.5 During the design of the field tests, the TSC recommended that sampling/analysis for HCL, PCDD's, PCDF's and metals not be done. This discussion was based on the lack of funding and time, and other needs of the project which necessitated Teflon™ coated glass fiber filters or quartz fiber filters. Metals could not be successfully assayed from these filters. Additionally the methodology and technology objectives of this study did not require the development of these data.

4.3.3.1.6 Accordingly the following sections do not address these issues.

4.3.3.1.7 Air Emissions

a. Gases

(1) Gas emissions for the mixed-manufacturing propellant waste burn carried out during the Phase B test series are given in Table 4.3.13. The measured CO₂ EF is 0.77 and, consistent with the other propellants examined in these tests, is within 1 percent of what one would expect to see if all the carbon in the propellant is converted to CO₂. The CO EFs are correspondingly low, and in the range of 10⁻³ to 10⁻⁴. The manufacturing residue, like the other propellants tested in this study, shows remarkably clean burning characteristics when burned in bulk quantities. Nitric oxide and nitrogen dioxide emissions for this propellant material were similar to those measured for the single- and triple-base materials discussed earlier, with levels in the range of 10⁻⁴ and 10⁻³.

b. Particulate Matter

Table 4.3.13 Gas Emission Factors for Phase B Manufacturing Residue Burns.

Species	Emission Factor (g/g)
CO ₂ - min	0.77
CO ₂ - max	0.77
CO ₂ - avg	0.77
Number of observations	9
CO - min	69 x 10 ⁻⁶
CO - max	1700 x 10 ⁻⁶
CO - avg	490 x 10 ⁻⁶
Number of observations	9
NO - min	1.9 x 10 ⁻³
NO - max	3.8 x 10 ⁻³
NO - avg	2.8 x 10 ⁻³
Number of observations	2
NO ₂ - min	0.34 x 10 ⁻³
NO ₂ - max	0.67 x 10 ⁻³
NO ₂ - avg	0.51 x 10 ⁻³
Number of observations	2

(1) The average particulate matter concentration as measured in several passes of the aircraft through the cloud from the Phase B manufacturing residue burn was 4.7 mg/m³. This concentration level is similar to those measured in the other propellant burn clouds. Assuming that all particles in the cloud are combustion products from the burn and that no soil is entrained into the smoke column during the burning process, the particulate matter EF corresponding to this cloud particle concentration level is about 1.6 percent. Thus, for every kilogram of propellant consumed, 16 grams of particulate material will be released to the atmosphere.

c. Volatile Organic Compounds

(1) Emission factors for VOC measured for the manufacturing residue are given in Table 4.3.14. Results are very similar to those determined for the M-30 triple-base material, in that only very low EFs (10⁻⁴) for the general class of TNMHC are detected; however, specific species such as CH₄ and benzene are not detected. These results are consistent with the observed general pattern of highly

efficient combustion of nearly all single-, double-, and triple-base propellants examined in this test program.

Table 4.3.14 Volatile Organic Compound Emission Factors, Phase B, Manufacturing Residue Burns.

Species	Emission Factor (g/g)
CH ₄ - min	BD*
CH ₄ - max	BD
CH ₄ - avg	BD
Number of observations	6
TNMHC - min	2.2×10^{-6}
TNMHC - max	230×10^{-6}
TNMHC - avg	45×10^{-6}
Number of observations	6
Benzene - min	BD
Benzene - max	BD
Benzene - avg	BD
Number of observations	6

*Below detection limit.

d. Semivolatile Organic Compounds

(1) Emission factors for the semivolatile organic category for the Phase B manufacturing residue burn are given in Table 4.3.15. Emission factors for most of the analytes on the target list are either nondetectable with a corresponding EF in the range of 10^{-6} to 10^{-9} , or are detected at a slightly higher level. The two analytes seen at the highest levels are naphthalene and phenol, with EFs in the 10^{-6} range. The pattern of semivolatile compound emissions from this propellant class is consistent with the emissions measured for the other single-, and triple-base propellants examined in this test series.

4.3.3.1.8 Soil Deposition

a. Sputter

Table 4.3.15 Semivolatile Organic Emission Factors, Phase B, Manufacturing Residue Burns.

Species	Emission Factor (g/g)
2,4-Dinitrotoluene	BD*
2,6-Dinitrotoluene	BD
2,4,6-Trinitrotoluene	BD
2-Nitronaphthalene	3.7×10^{-9}
N-Nitrosodiphenylamine	19×10^{-9}
Naphthalene	1500×10^{-9}
Benz[a]anthracene	38×10^{-9}
Benzo[a]pyrene	23×10^{-9}
Pyrene	71×10^{-9}
Phenol	8000×10^{-9}
Dibenzofuran	260×10^{-9}
Diphenylamine	20×10^{-9}

*Below detection limit which is less than 10×10^{-9} for most of the target analytes.

Ten sputter pan samples were placed 1 meter from the burn pans to collect propellant granules ejected from the burn pans during the burns. All propellant residue landing in the powdery soil or collected in the 1-m² pans visually appeared to be charred residue. This observation was substantiated by the low level of the analytes recovered. The mass of ash collected in the sputter pans averaged 2.8 g/m². The concentration of each analyte expressed as ng/g and ng/m² of terrain surface is given in Table 4.3.16.

Table 4.3.16 Summary of Semivolatile Analyte Concentrations, Phase B, Manufacturing Residue Burn, Sputter Pan Sampling.

Analyte	Number of Observations		Concentration Range	
	Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
Naphthalene	2	2	39 to 54	240 to 290
Pyrene	2	2	42 to 58	260 to 310
Phenol	2	2	0.65 to 0.77	4.0 to 4.1
Dibenzofuran	2	2	2.4 to 2.8	13 to 17
Nitroglycerin	2	2	22 to 23	120 to 130

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

b. Fallout

Fallout pan samplers were placed in concentric circles 6 and 12 meters from the center of the burn pan array. The mass of ash collected in the pans at 6 meters was 0.85 g/m². The mass of ash collected in the pans at 12 meters was 1.3 g/m². No sampling was conducted beyond 12 meters on the manufacturing residue burns; however, sampling beyond this distance on previous burns resulted in insufficient fallout for quantification of any of the analytes of interest. The analyte concentration data from the 6- and 12-meter fallout pans are summarized in Table 4.3.17. Using the maximum measured 2,4-dinitrotoluene concentration of 1300 ng/m² as representative of the terrain deposition out to 18 meters, results in a total deposition of 1.32 mg of 2,4-DNT, spread over 1000 m² or 0.25 acre.

Table 4.3.17 Summary of Semivolatile Analyte Concentrations, Phase B, Manufacturing Residue Burn, Fallout Pan Sampling.

Analyte	Sample Distance (m)	Number of Observations		Concentration Range	
		Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,6-Dinitrotoluene	6	2	2	100 to 700	170 to 1300
	12	2	1	BD ^d to 210	BD to 540
N-Nitrosodiphenylamine	6	2	0	BD	BD
	12	2	2	1.7 to 6.7	11 to 18
2-Nitrodiphenylamine	6	2	1	BD to 2.5	BD to 4.1
	12	2	2	13 to 17	34 to 110
Naphthalene	6	2	2	73 to 300	130 to 490
	12	2	2	160 to 390	1000 to 1000
Pyrene	6	2	2	67 to 510	120 to 840
	12	2	2	54 to 410	340 to 1100
Phenol	6	2	2	0.62 to 6.9	1.1 to 11
	12	2	2	8.1 to 16	41 to 50
Dibenzofuran	6	2	2	14 to 29	25 to 47
	12	2	2	5.4 to 16	33 to 41
Diphenylamine	6	2	1	BD to 2.7	BD to 4.5
	12	2	2	0.81 to 1.3	3.4 to 5.0
Nitroglycerin	6	2	2	76 to 100	140 to 170
	12	2	2	110 to 310	670 to 810

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

c. Burn Pan Residue

The amount of propellant burned was about 3000 kg on each burn. The burn pan residue amount varied from 3.4 kg to 7.4 kg or about 0.1 to 0.2 percent of the initial weight of propellant. The burn pan residue was analyzed by Chemtech, using EPA method 8270 (acid/base/neutral compounds), with the only compounds detected being phenol at 0.054 mg/kg of residue and the phthalates (phthalate compounds are not included on the semivolatile analyte list).

4.3.3.2 Manufacturing Residue Burn Test - Phase C

4.3.3.2.1 Air Emissions

a. Gases

Gas EFs for the mix of Navy NOSIH-AA-2 and N-5 manufacturing residues burned during Phase C test series are statistically summarized in Table 4.3.18. Minimum and maximum EFs are given for all significant gaseous species. Sample size was limited to four Teflon® bag samples for the NO and NO₂ species and about eight samples for CO₂, CO, and the VOC compounds. The minimum, maximum, and average CO₂ EF was observed to be 1.00 in all samples collected. This compares with a theoretical CO₂ EF of 1.00 for this particular propellant, assuming that all propellant carbon is converted to CO₂. The high CO₂ EFs are accompanied by very low (~ 0.0008) EFs for CO. This trend of high carbon conversion to CO₂ in these burns is consistent with observations made on the M-1 and M-6 single-base propellants as well. Nearly all of these propellants have a positive or near positive oxygen balance, so that little or no excess ambient air is required in the combustion zone to achieve complete conversion of carbon to CO₂. Nitrogen oxide emissions are at about the 0.1 percent level with nearly all of the gases in the NO category. These levels are consistent with those determined for the M-1 and M-6 propellant types discussed earlier. Assuming that all NO is ultimately converted to NO₂, the resulting NO₂ EF following NO oxidation is about 0.004 for this manufacturing residue.

Table 4.3.18 Gas Emission Factors for the Phase C Manufacturing Residue Burns.

Species	Emission Factor (g/g)
CO ₂ - min	1.00
CO ₂ - max	1.00
CO ₂ - avg	1.00
Number of observations	8
CO - min	0.005×10^{-3}
CO - max	3.0×10^{-3}
CO - avg	0.7×10^{-3}
Number of observations	8
NO - min	1.8×10^{-3}
NO - max	4.1×10^{-3}
NO - avg	2.6×10^{-3}
Number of observations	4
NO ₂ - min	22×10^{-6}
NO ₂ - max	600×10^{-6}
NO ₂ - avg	150×10^{-6}
Number of observations	4

*Below detection limit.

b. Particulate Matter

Particulate matter concentrations were measured twice during multiple aircraft passes through the plume. Each measurement represents an average of three cloud passages from two successive burns, starting at about 45 seconds and extending out to about 2.5 minutes after the completion of the burn. Gravimetric analysis of the particulate material collected on the filter and information on the air volume drawn through the filter provide a means of calculating the average cloud particulate matter concentration. Average cloud concentrations measured for August 14 and August 15 burns were 3.3 and 3.2 mg/m³, respectively. Concentration levels are consistent with low levels observed for other propellant types examined in these test series. These cloud concentrations correspond to a particulate matter EF of about 1 percent. Some existing evidence suggests that some of the particles in the cloud were soil particles entrained in the smoke column from the burning propellant; however, further testing is required to verify this theory.

c. Volatile Organic Compound

Emission factors for principal VOC compounds are given in Table 4.3.19 for the manufacturing residue test. Major species shown in the table include CH₄, TNMHC, and benzene. However all were detected at very low EF levels. Methane and TNMHC are both detected at slightly less than the 0.1 percent level and benzene is detected at the 0.01 percent level. These observations are similarly consistent with the low VOC emissions observed for the M-1 and M-6 propellant tests.

Table 4.3.19 Volatile Organic Compound Emission Factors for the Phase C Manufacturing Residue Burns.

Species	Emission Factor (g/g)
CH ₄ - min	3.8×10^{-6}
CH ₄ - max	3400×10^{-6}
CH ₄ - avg	750×10^{-6}
Number of observations	5
TNMHC - min	130×10^{-6}
TNMHC - max	1200×10^{-6}
TNMHC - avg	560×10^{-6}
Number of observations	7
Benzene - min	2.9×10^{-6}
Benzene - max	34×10^{-6}
Benzene - avg	16×10^{-6}
Number of observations	7

d. Semivolatile Organics (Exotics)

Emission factors for the semivolatile organic target compounds are given in Table 4.3.20 for the phase C manufacturing residue propellant burns. The values shown in the table are the maximum values obtained from two separate tests each consisting of two burns in series. Analysis allows the determination of thermally unstable compounds such as nitroglycerin which would otherwise decompose during injection and separation by conventional gas chromatography. The emission factors for the target analytes are all observed at the part per million (10^{-6}) level or less. The highest emission factors observed were for naphthalene, pyrene, and diphenylamine. Efficient combustion of the nitrodiphenylamine, present in the parent propellant at a level of 2 percent of the weight, is evidenced by an emission factor for diphenylamine of 3×10^{-7} . It is not likely that the

measured 2,4-dinitrotoluene, 2,6-dinitrotoluene, and 2,4,6-trinitrotoluene are derived from the chemical rearrangement of propellant constituents during the burn. It is noteworthy that nitroglycerin, one of the major propellant constituents, is not detected in the air samples collected. Similarly, the remainder of the target analytes were either not detected or observed at low (10^{-4} or 10^{-9}) levels.

Table 4.3.20 Maximum Semivolatile Organic Emission Factors Measured for the Phase C Manufacturing Residue Burns^a.

Species ^b	Emission Factor (g/g)
2,4 Dinitrotoluene	160×10^{-9}
2,6 Dinitrotoluene	140×10^{-9}
2,4,6 Trinitrotoluene	64×10^{-9}
2-Nitronaphthalene	83×10^{-9}
N-Nitrosodiphenylamine	27×10^{-9}
1,3,5-Trinitrobenzene	5.3×10^{-9}
2-Nitrodiphenylamine	13×10^{-9}
1-Nitropyrene	BD ^c
Nitroglycerin	BD
Naphthalene	540×10^{-9}
Benz[a]anthracene	140×10^{-9}
Benzo[a]pyrene	81×10^{-9}
Pyrene	320×10^{-9}
Phenol	--- ^d
Dibenzofuran	120×10^{-9}
Diphenylamine	310×10^{-9}

^aEmission factors are expressed in terms of 10^{-9} for ease of comparison, e.g., 160×10^{-9} is equivalent to 0.000000160.

^bSee Table 3.16 for a list containing the semivolatile organics and the detection levels.

^cBelow detection limit.

^d---Phenol was lost in the extraction of the semivolatiles.

4.3.3.2.2 Soil Deposition

a. Sputter

Ten sputter pan samples were placed 1 meter from the burn pans to collect propellant granules ejected from the burn pans during the burn. All manufacturing residue landing in the powdery soil or collected in the 1-m² pans visually appeared to be charred residue. This observation was substantiated by the low level of the analytes recovered. The mass of ash collected in the sputter pans averaged 3.2 g/m² on trial 1 and 1.8 g/m² on trial 2. The concentration of each analyte expressed as ng/g and ng/m² of soil surface is given in Table 4.3.21.

Table 4.3.21 Manufacturing Residue Burn: Summary of Semivolatile Organic Concentrations, Sputter Pan Sampling, Phase C.

Analyte	Number of Observations		Concentration Range	
	Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	2	2	5.5 to 21	15 to 58
2,6-Dinitrotoluene	2	2	1.8 to 8.1	4.9 to 22
2,4,6-Trinitrotoluene	2	1	BD ^d to 7.1	BD to 19
2-Nitronaphthalene	2	1	BD to 3.2	BD to 8.6
Naphthalene	2	1	BD to 13	BD to 34
Benz[a]anthracene	2	1	BD to 35	BD to 94
Benzo[a]pyrene	2	1	BD to 3.1	BD to 8.4
Pyrene	2	1	BD to 6.2	BD to 17
Dibenzofuran	2	1	BD to 30	BD to 80

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

b. Fallout

Fallout pan samplers were placed in concentric circles 6 and 12 meters from the center of the burn pan array. The mass of ash collected in the pans at 6 meters was 3.1 and 3.6 g/m² on trial 1 and trial 2, respectively. The mass of ash collected in the pans at 12 meters was 9.8 and 1.4 g/m² for trial 1 and trial 2, respectively. No sampling was conducted beyond 12 meters on the phase C manufacturing residue burns; however, sampling beyond this distance on previous burns resulted in insufficient fallout for quantification of any of the analytes of interest. The analyte concentration data from the 6- and 12-meter fallout pans are given in Table 4.3.22. Using the maximum measured

2,4-dinitrotoluene concentration of 24 ng/m² as representative of the terrain deposition out to 18 meters, results in a total deposition of 0.024 mg of 2,4-DNT spread over the 1000 m² or 0.25 acre.

Table 4.3.22 Manufacturing Residue Burn: Summary of Semivolatile Analyte Concentrations, Fallout Pan Sampling, Phase C.

Analyte	Sample Distance (m)	Number of Observations		Concentration Range	
		Total	AD ^a	(ng/g) ^b	(ng/m ²) ^c
2,4-Dinitrotoluene	6	2	2	7.3 to 7.5	11.4 to 11.8
	12	2	2	3.7 to 23	3.9 to 24
2,6-Dinitrotoluene	6	2	2	4.3 to 5.0	6.8 to 7.9
	12	2	2	0.62 to 4.8	0.65 to 5.1
2,4,6-Trinitrotoluene	6	2	0	BD ^d	BD
	12	2	2	0.62 to 120	0.64 to 120
2-Nitronaphthalene	6	2	2	2.3 to 5.0	3.7 to 7.9
	12	2	2	0.42 to 8.4	0.44 to 8.8
1,3,5-trinitrobenzene	6	2	0	BD	BD
	12	2	1	BD to 5.4	BD to 5.7
Naphthalene	6	2	1	BD to 11	BD to 18
	12	2	1	BD to 23	BD to 24
Benz[a]anthracene	6	2	1	BD to 7.8	BD to 12
	12	2	1	BD to 29	BD to 30
Benzo[a]pyrene	6	2	1	BD to 1.7	BD to 2.7
	12	2	1	BD to 0.079	BD to 0.083
Pyrene	6	2	1	BD to 3.0	BD to 4.6
	12	2	1	BD to 15	BD to 16
Dibenzofuran	6	2	0	BD	BD
	12	2	1	BD to 48	BD to 50
Diphenylamine	6	2	0	BD	BD
	12	2	1	BD to 21	BD to 21

^aAbove detection limit.

^bRepresents ng of analyte per gram of fallout.

^cRepresents ng of analyte per m² of terrain.

^dBelow detection limit.

c. Burn Pan Residue

Burn pan residue for each 2200 kg of manufacturing residue burned varied from 0.37 kg to 1.1 kg over the four burns. The average residual was 0.61 kg, or about 0.03 percent of the initial weight

of propellant. Burn pan residue samples for semivolatile organic analyses were taken on each burn. A composite sample for each of the burn trials was analyzed. The semivolatile organic analytes detected and the concentrations are given in Table 4.3.23.

Table 4.3.23 Manufacturing Residue Burn: Summary of Semivolatile Analyte Concentrations, Burn Pan Residue, Phase C.

Analyte	Number of Observations		Concentration Range (ng/g) ^b
	Total	AD ^a	
2,4-Dinitrotoluene	2	2	1.8 to 6.0
2,6-Dinitrotoluene	2	2	3.5 to 5.0
2-Nitronaphthalene	2	2	0.13 to 3.6
Benzo[a]pyrene	2	2	11 to 11
Pyrene	2	2	3.2 to 5.2
Dibenzofuran	2	2	18 to 22
Diphenylamine	2	1	BD ^c to 1.9

^aAbove detection limit.

^bRepresents ng of analyte per gram of pan residue.

^cBelow detection limit.

4.4 Comparison of BangBox and Field TNT Detonations

EFs from the BangBox, open-air *surface*, and open-air suspended TNT detonations are summarized in Table 4.4.1. This table gives values for CO₂, CO, NO, NO₂, volatile organics, (methane, TNMHC, and benzene), and the selected list of semivolatiles.

Table 4.4.1 Average Emission Factors for the Volatile and Maximum Emission Factors for the Semivolatile Analytes from the BangBox and Open-Air Detonation with TNT.

Analyte	BangBox	Phase A Surface	Phase B		Phase C	
			Surface	Suspended	Surface	Suspended
CO ₂	1.32	1.26	1.29	1.35	1.28	1.35
CO	4.9×10^{-3}	61×10^{-3}	42×10^{-3}	7.3×10^{-3}	49×10^{-3}	6.9×10^{-3}
NO	11×10^{-3}	0.70×10^{-3}	1.4×10^{-3}	2.5×10^{-3}	1.4×10^{-3}	2.3×10^{-3}
NO ₂	0.56×10^{-3}	3.6×10^{-3}	1.1×10^{-3}	2.1×10^{-3}	1.4×10^{-3}	1.2×10^{-3}
Methane	0.025×10^{-3}	1.5×10^{-3}	1.2×10^{-3}	0.061×10^{-3}	1.5×10^{-3}	1.5×10^{-3}
TNMHC	0.057×10^{-3}	1.4×10^{-3}	1.9×10^{-3}	0.21×10^{-3}	2.1×10^{-3}	5.0×10^{-3}
Benzene	2.4×10^{-6}	94×10^{-6}	93×10^{-6}	3.2×10^{-6}	100×10^{-6}	62×10^{-6}
2,4-DNT	170×10^{-9}	150×10^{-9}	8400×10^{-9}	200×10^{-9}	BD ^a	BD
2,6-DNT	140×10^{-9}	19×10^{-9}	7100×10^{-9}	300×10^{-9}	BD	BD
2,4,6-TNT	620×10^{-9}	220×10^{-9}	150×10^{-9}	46×10^{-9}	60×10^{-9}	140×10^{-9}
2-NN	160×10^{-9}	80×10^{-9}	270×10^{-9}	15×10^{-9}	BD	BD
N-NSDPA	200×10^{-9}	BD	4.4×10^{-9}	29×10^{-9}	BD	BD
1,3,5-TNB	0.45×10^{-9}	BD	BD	BD	BD	BD
2-NDPA	N/A ^b	N/A	N/A	N/A	BD	BD
1-NP	1/13 ^c	BD	39×10^{-9}	59×10^{-9}	BD	BD
Naph	28×10^{-6}	BD	3.7×10^{-6}	0.012×10^{-6}	2.6×10^{-9}	1.8×10^{-9}
B[a]A	BD	2.2×10^{-9}	160×10^{-9}	66×10^{-9}	100×10^{-9}	320×10^{-9}
B[a]P	360×10^{-9}	BD	240×10^{-9}	310×10^{-9}	BD	BD
Pyrene	32×10^{-9}	BD	NA	N/A	220×10^{-9}	19×10^{-9}
Phenol	9.9×10^{-6}	BD	5.2×10^{-6}	12000×10^{-6}	BD	BD
DBF	150×10^{-9}	BD	85×10^{-9}	60×10^{-9}	180×10^{-9}	190×10^{-9}
DPA	BD	N/A	7.7×10^{-9}	25×10^{-9}	170×10^{-9}	BD

^aBelow detection limit.

^bN/A - Not on the analyte list.

^cDetected on one of 13 assays, at very low level.

4.4.1 Emission Factor Comparison.

Changes in the EF for any particular species would not be expected if the explosive configuration (suspended or surface) or the size of the detonation has no effect on the amount of the pollutant produced, since the EF is the amount of pollutant released, normalized to the original mass of

material. The EF for several of the gases reveals that either scale or configuration effects are operative. For example, the CO₂ EF is higher for the BangBox and suspended outdoor tests when compared to those from the outdoor *surface* detonations. Since the small-scale BangBox and large-scale suspended EF for CO₂ are similar, it can be surmised that the suspended configuration of the explosive is an important parameter in the CO₂ formation process. As discussed earlier, the presence of entrained soil debris in the detonation fireball during the *surface* tests is believed to depress the fireball temperature, as well as limit the degree of entrainment of ambient air into the fireball. Similar EF discontinuities can be noted for CO, CH₄, and TNMHC species when the BangBox and suspended tests are compared to the *surface* tests. Differences in the semivolatile target analyte EFs from BangBox, suspended, and *surface* TNT tests are less pronounced when compared to those of the gaseous products. The semivolatile category of emission products appears to be least influenced by explosive configuration or scale. These results suggest that small-scale, low cost experiments may be useful in the determination of pollutant releases, if the EF scale effects for some of the less-toxic gaseous species can be appropriately considered at the smaller scales.

4.4.2 Comparison of Carbon Distribution.

The fate of TNT carbon for all TNT test categories is summarized in Table 4.4.2. Here, an average of the mass fraction of carbon released as CO₂, CO, CH₄, TNMHC, particulate organic carbon (OC), and particulate elemental carbon (EC) is shown for the BangBox, *surface*, and suspended TNT detonations. As noted in the results section for each test configuration, the majority of the carbon goes to CO₂. In all cases, the CO₂ category receives in excess of 92 percent of the original TNT carbon. Allotments to the CO₂ category are highest for detonations carried out in the absence of soil and are lowest for those done in close contact with soil. With a few exceptions, each of the other two emission categories (EC and OC) receive about 1 percent of the original carbon. A notable exception is the CO category in the *surface* tests, which receives about 5 percent of the original carbon mass. The particulate organic carbon category for the open air-tests is a worst-case estimate as it appears in this table, since measurements of local Dugway soil reveal a significant particulate organic carbon component in the soil. Distinguishing between soil-derived and TNT-derived particulate OC is not attempted here. However, soil analysis results suggest that nearly all the carbon in the OC category may originate from soil entrained in the cloud. This is not the case with particulate EC, category since soil analysis shows nondetectable levels of EC.

Table 4.4.2 Distribution of Carbon Emissions by Pollutant Category for BangBox and Open-Air Surface and Suspended TNT Detonations.

Species ^a	Mass Fraction of Carbon Released					
	BangBox	Phase A Surface	Phase B Surface	Phase C Surface	Phase B Suspended	Phase C Suspended
CO ₂ (gas)	0.977	0.950	0.920	0.936	0.983	0.974
CO (gas)	0.006	0.013	0.053	0.056	0.008	0.008
CH ₄ (gas)	BD ^b	0.014	0.002	0.003	BD	0.005
TNMHC (gas)	BD	0.009	0.004	0.003	BD	0.013
OC ^c (particles)	0.0001	0.007	0.014	N/M ^d	0.0001	N/M
EC ^e (particles)	0.017	0.008	0.007	N/M	0.017	N/M

^aIn all cases, the carbon mass fraction release to the compounds included in the semivolatile organic target analyte list is less than 5×10^{-3} .

^bBelow detection limit.

^cAn analysis of Dugway soil suggests that nearly all the particulate organic carbon (OC) detected in the cloud may be attributable to suspended soil. Here, it is conservatively assumed that all detected OC is an emission product from the TNT detonation and is not corrected for soil contributions.

^dN/M - Measurement for the species of carbon not made.

^eElemental carbon.

4.5 Dispersion Model Screening Analysis

4.5.1 Dispersion modeling has been extensively used to estimate downwind pollutant concentrations that would arise from either a continuous or instantaneous release of pollutants from a point source. An analysis was carried out using the DPG volume source dispersion model RTVSM (Reference 7) and a range of EFs measured for surface TNT detonations during the OB/OD tests. This particular model uses simple Gaussian dispersion calculations to estimate maximum and timed average ground level concentrations. The stable cloud radius was derived using Briggs plume rise techniques (References 8 and 9) which specify that the cloud radius expands linearly at a factor of 0.64 of the cloud height for an instantaneous source. Results can be used to assess potential exposure hazards that personnel in the region of cloud impact with the ground might encounter. Three release scenarios were selected for dispersion analysis that reflect downwind concentrations of three general classes of pollutants. These include (1) criteria gases such as CO; (2) VOC species such as benzene; and, (3) semivolatile organic compounds such as benzo[a]pyrene. Input assumptions for each of the three cases are given in Table 4.5.1. An initial

explosive mass of 1 metric ton (1,000 kg) was used in all model cases along with a stabilized cloud height estimate of 330 m. The cloud height estimate represents a conservative estimate in good agreement with *minimum* stabilized cloud heights actually observed during aircraft sampling of detonation clouds during the various testing phases. This cloud height estimate represents a worst case analysis from the perspective of predicting ground level concentrations since the lower (minimum) cloud height will yield higher ground level concentrations.

Results from the three cases selected are shown Table 4.5.1 with Figure 4.1 showing an output plot of the RTVSM model for CO. Maximum peak instantaneous and maximum 15-minute average ground level concentrations for each of the three cases examined are at low levels. For example, surface detonation of 1 metric ton of TNT would result in peak ground level CO concentrations of $210 \mu\text{g}/\text{m}^3$ or about 0.18 ppm. These levels are insignificant in light of the fact that rural "clean air" background CO levels are typically in the vicinity of 0.1 ppm. A similar result occurs for benzene. Where the model predicts downwind peak instantaneous benzene concentrations of $0.43 \mu\text{g}/\text{m}^3$, actual background levels in "clean air" are in the range of 0.5 to $1.5 \mu\text{g}/\text{m}^3$. The background benzene concentration level is thus nearly the same as that arising from a TNT detonation as predicted by this dispersion model. The semivolatile case reveals even lower peak instantaneous ground concentration levels in the vicinity of $0.43 \text{ ng}/\text{m}^3$. Typical polynuclear aromatic hydrocarbon concentrations such as benzo[a]pyrene are encountered in "clean air" at concentration levels ranging from 0.01 to $0.40 \text{ ng}/\text{m}^3$ (Reference 10). Here again, benzo[a]pyrene pollutant contributions at downwind ground level locations are in the same range as clean air ambient background concentrations and would not be distinguishable from clean air background levels. Of particular note is the fact that 15 minute average downwind concentrations as "seen" by a ground level receptor at a fixed point during passage of a single diluted puff are lower than the peak instantaneous values by about a factor of ten. Since most personnel exposure criteria are based on exposure intervals of 15 minutes or longer, these levels are more representative of potential downwind exposure levels that may be encountered. These dispersion model results strongly suggest that air emissions from these large scale detonations pose no health threat to personnel downwind of the cloud.

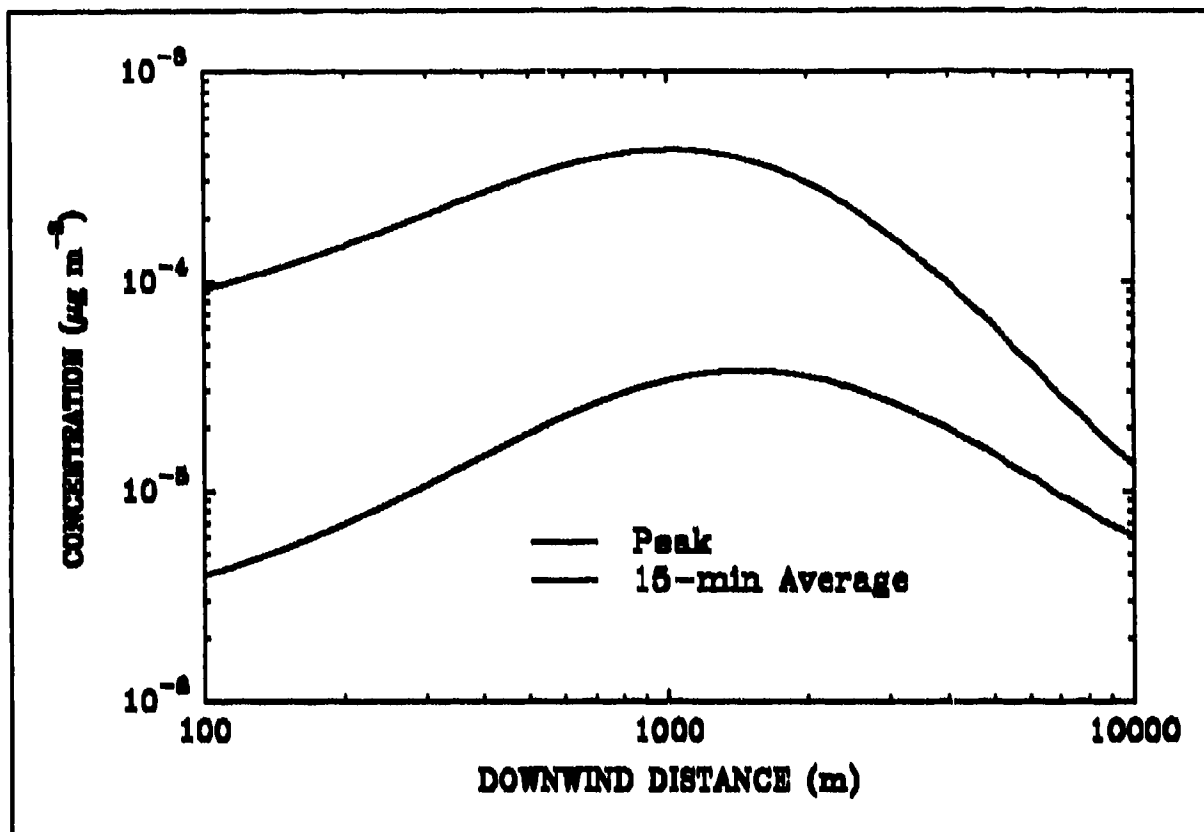


Figure 4.1 Ground Level Peak and 15 min Average Concentration of Benzo[a]pyrene Downwind of a 1000-kg Surface Detonation of TNT.

Table 4.5.1 Input Data and Downwind Ground Level Pollutant Concentrations for Selected Cases Using the DPG Volume Source Dispersion Model.

Input/Output Parameter	Case 1 Gas (CO)	Case 2 VOC (Benzene)	Case 3 Semi-volatile (Benzo[a]Pyrene) ^a
EF	5×10^{-2}	1×10^{-4}	0.1×10^{-6}
Total Release (kg) ^b	50	0.1	0.0001
Stable Cloud Height (m)	330	330	330
Stable Cloud Radius (m)	211	211	211
Wind Speed (m/s ¹)	5	5	5
Stability Class	Unstable	Unstable	Unstable
Max Downwind Inst. Conc ^c ($\mu\text{g}/\text{m}^3$)	210	0.43	0.00043
Max 15 min Avg Conc ^d ($\mu\text{g}/\text{m}^3$)	19	0.038	0.000038
Downwind range for peak conc (km)	1	1	1
Downwind range for avg conc (km)	1.5	1.5	1.5

^aBenzo[a]pyrene was only found on the TNT detonations during Phase B test.

^bTotal pollutant release is based on a 1000 kg surface detonation of bulk TNT and an assumption that all of the compound becomes an air emission. This is essentially true for Case 1 and Case 2 but is approximately a 2 order of magnitude over estimate for Case 3 (semi-volatile).

^cMaximum downwind instantaneous concentration at ground level.

^dMaximum downwind 15 minute average concentration at ground level.

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SECTION 5. SUMMARY OF QA ACTIVITIES FOR OB/OD PROGRAM

5.1. Overview

5.1.1. The OB/OD program was conducted in four phases, a controlled chamber test (BangBox), and three field tests (Phases A, B, and C).

5.1.2. The purposes of the BangBox tests were (1) to characterize the emission products resulting from OB/OD operations, (2) to evaluate candidate sampling and analysis methods for measuring these emission products, and (3) to develop the QA and QC procedures necessary to ensure that the program met its data quality objectives.

5.1.3. Field Test Phase A was a pilot test to evaluate the candidate sampling and analysis techniques selected from the results of the BangBox tests. Field Test Phases B and C were full-scale field tests to assess the impact of OB/OD activities on the environment and to determine if BangBox-type tests adequately simulate the emission products from real world OB/OD operations.

5.1.4. All organizations making measurements in the OB/OD project were expected to have either standard operating procedures (SOP's) or letters of instruction (LOI's) for each phase of the program. Two organizations, SSL and OGC, did not have approved LOI's in place until after the BangBox tests were completed. However, these organizations are very small and one principal analyst handles all the samples. In the view of all auditors, the lack of an approved LOI did not affect the quality of the analyses provided by these two organizations. The SOP's and LOI's were revised as the program progressed and the measurement methods were improved or revised.

5.1.5. A quality assurance project plan (QAPP) containing the SOP's and LOI's was developed for each phase of the program. The QAPP described the quality control (QC) activities that would be followed by the organizations making measurements in that phase of the program. Sample QC activities used in the OB/OD program were (1) matrix spikes, (2) method of standard additions, (3) replicates, (4) split samples, (5) sample chain-of custody, (6) up to date and readable laboratory logbooks, and (7) preventive maintenance on the equipment.

5.1.6. Two organizations were responsible for the external QA, ELI (Provo, Utah) and U.S. Environmental Protection Agency Atmospheric Research and Exposure Assessment Laboratory (USEPA/AREAL) Quality Assurance Division (Research Triangle Park, NC).

5.1.6.1. ELI, the contract QA organization for AMCCOM conducted quality systems audits (QSA) on all organizations making measurements to provide a qualitative assessment of the conformance of the organization to their QC procedures and to its LOI's/SOP's. The ELI QSA's addressed the following: (1) LOI status, (2) field/laboratory sampling, (3) field/laboratory analysis, (4) instrument/method calibration, (5) preventive/corrective maintenance, (6) internal QC procedures, (7) sample preparation and storage, (8) preparation and use of spiked samples, (9) instrument/equipment selection and use, (10) determination of detection limits/limits of quantification, (11) sample handling and transportation, (12) data reduction and analysis, (13) logbooks, (14) personnel working with samples, (15) building diagrams, (16) research journals, (17) tracking system for samples, and (18) overall assessment/recommendations and comments.

5.1.7. The USEPA audit team conducted QSA's and quality performance audits (QPA's) on the organizations making measurements. QPA's provide a quantitative assessment of an organization's performance by challenging their measurement system with accurately prepared samples which have levels or values that are unknown to the organization being audited. These EPA QPA's included checks on the following: (1) Sample flow-rate accuracy, (2) Carbon monoxide, carbon dioxide, nitrogen oxide, nitrogen dioxide, ozone, and sulfur dioxide air monitor accuracy, (3) percent recovery of semivolatile organic compounds (SVOC's) from soil, particulate, and canister samples, and (4) percent recovery of VOCs from canisters.

5.1.8. Appendix J provides an "in-depth" description of the procedures used for the QSA's and QPA's, the findings of the QSA's, QPA's, and corrective actions taken by the audited organization, and the auditors' assessment of the impact of the findings on the data quality. Tables 5.1 and 5.2 reveal when and by whom QSA's and QPA's were conducted.

5.1.9. A summary of the findings by measurement type and, where appropriate, an assessment of the findings on the data quality of the OB/OD thermal treatment program is provided below.

5.2. Inorganic Gases (Carbon Monoxide, Carbon Dioxide, Nitrogen Oxide, Nitrogen Dioxide, Sulfur Dioxide, Ozone) Measured by Continuous Monitors

5.2.1. All monitors (including the associated data collection system) were operating within an accuracy of ± 10 percent (the data quality goal for the program), with the exception of the carbon dioxide monitor in phase A. This later monitor was reading high by 14 percent, because the zero had shifted. However, this shift did not affect the use of the measurement, because the carbon dioxide measured before the plane entered the plume was subtracted from the carbon dioxide measured in the plume. Since the baseline shift affected both measurements equally, the amount of carbon dioxide formed from the detonation was accurately measured. SNL recalibrates the monitor as soon as the shift in baseline is detected. The logbooks were kept current and SRMs (standard reference materials from the National Institute for Standards and Technology (NIST)) were used to calibrate the carbon monoxide, carbon dioxide, nitrogen oxide, and sulfur dioxide instruments. Since there are not SRM's for nitrogen dioxide or ozone, these instruments were calibrated with transfer standards traceable to the NIST.

5.2.2. Two problems occurred throughout the OB/OD program. The auditors continually found that SNL did not have spare parts for the monitors on the aircraft, and SNL failed to check out the monitors before the aircraft left Albuquerque. While these problems did not affect the quality of the data, they did cause extensive delays during the field tests. Sometimes a full day's testing was canceled because one or more of the monitors was not operating and the required spare part was not available on site.

5.3. Flow Rate of Particulate and VOST Samplers

5.3.1. Particulate Sampler

The flow-rate through the aircraft's sampling probe was checked at the probe inlet during the three field tests and determined to be within the ± 5 percent of the reference flow. This was within the ± 10 percent data quality objective for the OB/OD project.

5.3.2. VOST Sampler

The sampler was used only in the BangBox tests. All samplers had flow-rates within 7 percent of the reference standard.

5.4. Volatile Organic Samplers

5.4.1. During all four phases of the program 6-L canisters provided to EPA by OGC were spiked with known quantities of VOCs by EPA at 1 to 5 ppb. The canisters were then returned to OGC. The percent recoveries achieved by OGC for the OB/OD target compounds were consistently excellent and well within the 75- to 125-percent target range. Precision was also excellent, generally less than 5-percent RSD.

5.4.2. QSA's were completed on the VOC sampler in the BangBox test, the three field tests, and also in the OGC laboratory. No deficiencies that would affect data quality were found. During Phase A and once in Phase C, the inlet valve to the canister's sampling manifold failed to open. In these cases the samples were voided.

5.5. Semivolatile Organic Samplers

5.5.1. 32-L Tanks with Filters on Inlet

This sampler was used in the BangBox test in an attempt to simultaneously collect large VOC and semivolatile organic compounds (SVOCs) samples. The SVOC's were expected to be collected on the filter and also in the tanks. EPA placed known quantities of seven SVOC's in the tanks and sent them to BCD and to AWL for extraction, and subsequent analysis for SVOC's. Recoveries of all seven compounds were less than 50 percent, the OB/OD program's lower limit for SVOC analysis. The audit results showed that this was not a viable sampler for the program and it was dropped from the program before the field tests were begun.

5.5.1.1. QSA's by EPA and ELI showed that both laboratories followed the LOI for the method and that the sampler was leak-free prior to use in the BangBox tests.

5.5.2. Semivolatile Organic Sampling Train Sampler

5.5.2.1. This sampler, which used a filter followed by XAD-2^o cartridges to collect SVOC's, was used in the BangBox tests in an attempt to collect large quantities of SVOC. EPA placed known quantities of seven SVOC's on XAD-2^o sampling cartridges and sent them to BCD and AWL for extraction and analysis. A solution containing the same seven SVOC's accompanied the cartridges to serve as a benchmark measure on the analytical portion of the method. BCD achieved recoveries between 70 and 135 percent for the solution, but recovered less than 50 percent for three of the seven compounds placed on the XAD-2^o. AWL achieved less than 50-percent recovery for all seven compounds. It was subsequently determined that the XAD-2^o had been heated too long during cleanup prior to use, and all samples were then voided. The VOST sampler was dropped from the program before field tests were begun, because the BangBox tests and the open literature indicated that a high-volume filter would be adequate for collecting SVOC's. The QSA's determined that BCD and AWL followed the LOI for the extraction and analysis of the samples.

5.6. SVOCs Particulate from Sampler (Aircraft) and Fallout Pans

5.6.1. The material collected on the filter and in the fallout pans from detonations was expected to be mostly soil particles containing some SVOC's. EPA placed known quantities of SVOC's on background soil samples from DPG, and these were then extracted and analyzed by AWL. The first spiked soil samples (BangBox Test) contained 5 to 36 μg of seven SVOC's. AWL achieved quantitative recovery for all seven SVOC's using both SFC-MS and GC-MS. For Phase A, no spiked soil samples were used because the objective was to check out the sample collection procedures developed from the BangBox tests. Spiked soil samples were used in Phases B and C, however, where ancillary tests were also done to evaluate the spiking and analytical methods being used in the OB/OD project.

5.6.1.1. Nanogram rather than μg quantities of analytes were used for Phases B and C because the BangBox test results showed that only ng quantities of analytes would likely be encountered in the soil samples from the field test. The analytes spiked on the soil samples in Phases B and C were somewhat different from those used in the BangBox spiked soil samples, i.e., 1-nitropyrene, dibenzofuran, pyrene, 1,3,5-trinitrobenzene, 2,6-dinitrotoluene, 2,4-dinitrotoluene and naphthalene were added and N-nitrosodiphenylamine and the two nitrophenols were deleted from the original list.

5.6.1.2. Low recoveries (less than 50%) were found for all analytes for the Phase B soil sample spikes; these low recoveries were subsequently determined to have resulted from reduced sensitivity of the SFC-MS used to analyze the extracts. The reduced sensitivity resulted from the chromatographic coating being striped from the SFC's column by the acetonitrile carrier and being carried to the MS's quadrapole area where it deposited. The SFC-MS unit was repaired for the Phase C samples and acceptable recoveries were achieved for the analytes except phenol, 1,3,5-trinitrobenzene, 2,6-dinitrotoluene and naphthalene. The samples used for Phase C were spiked using two established methods, the slurry/rotary evaporator technique and the aluminum (foil) roll technique to see if the spiking technique affected the recovery of the analytes from the soil. In the slurry technique the solvent (100 - 200 ml per 400 grams of soil) is removed at elevated temperatures (45-80°C) using a rotary evaporator. There was concern that some of the more labile analytes would be lost. In contrast, the aluminum roll technique lets the solvent (1 ml) air-evaporate. Five soil samples were spiked by the slurry technique and five were spiked by the aluminum roll techniques. The samples were spiked with the same quantities of analytes. All extracts were analyzed by GC-MS and SFC-MS to also determine if the GC-MS and SFC-MS gave equivalent results.

5.6.2. The results of these tests (based on the percent of the analyte recovered from the soils) were:

5.6.2.1. There was no difference in soils spiked by the aluminum roll and those spiked by the slurry/rotary evaporator technique.

5.6.2.2. Phenol was not recovered from any sample. Therefore, phenol should not be used as a target analyte at least if a Soxhlet extraction procedure is used. Whether phenol would be recovered if a sonification technique is used for extraction is unknown.

5.6.2.3. Consistently low recoveries were obtained for diphenylamine. This is expected because amines are tightly bound to soils. Low recoveries were also found in many samples for 1,3,5-trinitrobenzene, 2,6-dinitrotoluene and naphthalene.

5.6.2.4. Samples that were not spiked showed small quantities of 1,3,5-trinitrobenzene and 2,4-dinitrotoluene. This indicated either previous contamination of the soil sample before it was received for spiking or the presence of an interfering ion.

5.6.2.5. The results showed that the analytes can be quantitatively transferred to dichloromethane from the acetonitrile used to extract the analytes from the soil. This is encouraging because it provides a means to remove the acetonitrile solvent before the sample is placed in the SFC-MS system. (Acetonitrile was found to dissolve the gas chromatographic column's stationary phase which caused the column material to enter the MS unit.)

5.6.3. At this time, there are no reference soil samples that contain accurately known recoverable quantities of SVOC's, so the overall accuracy of the extraction and analysis of the DPG soil samples for SVOC's is uncertain. However, AWL obtained the precision normally expected for soil analyses when they extracted and analyzed duplicate field samples and when they reanalyzed extracts from soil samples months after the original analyses.

5.6.4. Quality system audits on AWL when they were extracting and analyzing soil and filter (particulate) samples showed that they were properly calibrating the SFC-MS unit and using the extraction technique in the LOI. Record keeping was a continual problem but in each instance the problems were corrected and it is felt that no samples were misidentified. AWL is a small research laboratory with one principle analyst and it is not accustomed to employing the labor-intensive sample tracking system normally used by laboratories that provide routine analytical services.

5.7. Metals by XRF

5.7.1. Only QSA's were performed, since LBL uses NIST certified calibration standards. Metals analyses (19 metals) were done on samples from the BangBox and from Phase C. The QSA's determined that the laboratory consistently achieved precision of ± 6 percent or better on its QC samples, well within their ± 10 percent QC goals. If the ± 10 percent QC target goal was exceeded, the analysis was voided and the sample was reanalyzed after the instrument was recalibrated. LBL is essentially a three-man operation with one principal analyst. They employ an EPA-approved analytical method.

5.8. Elemental and Volatilizable Carbon

Only QSA's were conducted on the carbon measurement system, because SSL was employing a comprehensive QC program. Sucrose samples placed on filters and rods containing accurately known quantities of carbon containing compounds were used for calibration and for QC checks. The QSA's revealed no deficiencies or deviations from the LOI.

5.9. Real Time Particle Measurements (Aircraft)

Only QSA's were conducted on the two particle counters employed on the aircraft, because there are no field-proven calibration/auditing systems. Both instruments were calibrated against NIST standards less than one year before the field tests, which met the date quality goal. These instruments were used primarily to detect entry into and exit from the plume, and no particle concentration calculations were attempted.

5.10. HCN, NH₃, HCL Samplers

These samplers, which employed impingers, were used in the BangBox tests. Measurable quantities of the three compounds were not detected in the BangBox, and the use of the sampler was discontinued. The QSA showed that the published reference method was followed for sampling and analysis and that certified calibration standards were used to calibrate the colorimeter.

5.11. Fallout and Burn Pan Sampler Placement and Recovery

Extensive QSA's were performed by EPA and ELI during all three field tests. No major deficiencies or deviations from the LOI's were found that would impact on the quality of the data. The Lockheed Engineering and Sciences Company (LESC) personnel were observed to be well-trained, conscientious, and very proficient in executing their duties. No cases of sample misidentification were detected, and all samples were taken in accordance with the LOIs.

5.12. Particulate Weight Determination

5.12.1. The particulate sample filters from the BangBox and phases A and B were transported to AWL for conditioning and particulate weight determination. The filters from Phase C were conditioned and weighed at DPG by SNL. The decision was made to weigh the Phase C filters at DPG to reduce the chance that particulate would be lost from the filters during transport and to provide improved facilities for filter conditioning.

5.12.2. QSA's did not detect any instances where samples were misidentified, or the particulate contaminated or lost after collection. However, AWL's record-keeping system was cumbersome to follow, because the logbook was organized by date and not by sample number. Since the filters were weighed at periodic intervals over several days (until a constant weight was obtained) the auditor had to check numerous pages to determine how many times a specific filter was weighed and the change in weight between determinations.

Table 5.1 **Schedule of Quality System Audits During OB/OD Program**

Audited Organization	Test Phase	Auditing Organization	
		ELI	EPA
Battelle-Columbus	BangBox	28 Dec 88	NA ^a
Oregon Graduate Center	BangBox	24 Jan 89	NA
	Phase B	18 Jan 90	7 Nov 89
Sunset Laboratory	BangBox	23 Jan 89	NA
	Phase A	9 May 89	NA
	Phase B	17 Jan 90	NA
Lawrence Berkeley Laboratory	BangBox	31 Jan 89	NA
Brigham Young University (PIXE ^b Lab)	Phase B	14 Feb 90	21 Feb 90
Lockheed Engineering and Science Co.	Phase C	6-19 Aug 90	6-27 Aug 90
			20 Feb 90
Environmental Laboratories Inc.	Phase C	NA	6-27 Aug 90
Sandia National Laboratories	BangBox	16-17 Dec 88	30 Nov-2 Dec 88
			Feb 89
	Phase A	NA	Jun 89
	Phase B	13-19 Oct 89	13-27 Oct 89
	Phase C	NA	6 Aug- 19 Sep 90
Alpine West Laboratories	BangBox	18 Jan 89	NA
	Phase A	17 Jul 89	NA
	Phase B	9 Feb 90	19, 24 Oct 89
			5-6 Dec 89
			20-21 Feb 90
	Phase C	NA	16 Aug 90
			15 Nov 90

^aNot applicable, QSA not conducted by ELI or EPA.

^bParticle Induced X-ray emission.

Table 5.2 **Schedule of EPA Quality Performance Audits During OB/OD Program.**

Audited Organization	Test Phase	Audit Dates	Measurement Parameters or Analyte Involved
Sandia National Laboratories	BangBox	6-8 Feb 89	Flow rate: particulate samplers, XAD cartridge sampler. Gas analyzers: CO, CO ₂ , O ₃ , SO ₂ , NO, NO ₂ .
	Phase A	Jun 89	Gas analyzers: CO, CO ₂ .
	Phase B	Oct 89	Flow rate: aircraft probe.
			Gas analyzers: CO, CO ₂ , O ₃ , SO ₂ .
	Phase C	6-10 Aug 90	Flow rates. Gas analyzers: CO, CO ₂ , O ₃ , NO, NO ₂ .
Alpine West Laboratories	BangBox	Dec 88	Spiked soil, spiked XAD-2 cartridges. Spiked 32-L tank.
	Phase B	Nov 89	Spiked soil.
	Phase C	Dec 90	Spiked soil.
Battelle-Columbus Division	BangBox	Dec 88	Spiked soil, spiked XAD-2 cartridges. Spiked 32-L tank.
Oregon Graduate Center	BangBox	Dec 88	Spiked 6-L canisters.
	Phase B	Nov 89	Spiked 6-L canisters.
	Phase C	Aug 90	Spiked 6-L canisters.

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SECTION 6. CONCLUSIONS

6.1. Background

6.1.1. BangBox

The BB conclusions are stated in the BB report, Volume 1.

6.1.2. Field Test Phase A

6.1.2.1. Purpose

Field Test Phase A was designed as a program ORI.

6.1.2.2. Objectives

6.1.2.2.1 Objective 1 - Evaluate the performance of the instrumented FWAC as a sampling platform during large-scale field OB/OD tests.

a. The FWAC proved to be a suitable sampling platform. The aircraft's design enabled the aircraft to enter and sample the plume within approximately 1 min after the detonation, and make repeated penetrations of the plume. The sampling passes made through the cloud permitted real-time analyses of some gases and captured sufficient quantities of gases and particulates for subsequent analyses.

b. Additionally the instruments and procedures used on the FWAC were judged suitable for subsequent testing.

6.1.2.2.2 Objective 2 - Determine if target species can be adequately sampled and measured above background levels.

a. Carbon dioxide and other target species were adequately sampled and measured above background levels using real-time instruments aboard the FWAC.

b. The VOC's were successfully measured above background levels with the 6-L canister sampler. Carbon dioxide and CO were also successfully measured above background with the 6-L canister.

c. The quartz fiber filters collected sufficient particulate for the detection and quantification of SVOC's.

6.1.2.2.3 Objective 3 - Evaluate the utility of the carbon balance method in the field testing environment.

The utility of the carbon balance method was confirmed. The FWAC ability to enter the plume and measure CO₂ well above background supports the carbon balance method applicability to field testing.

6.1.2.2.4 Objective 4 - Evaluate soil sampling, handling, and assay procedures (e.g. SFC/MS) for field OB/OD tests.

Soil sampling, handling, and assay procedures were proven suitable for capturing and analyzing emittant products released into the soil during field testing.

6.1.3. Field Test Phase B

6.1.3.1. Purpose

Confirm suitability of instruments and procedures developed in Phase A, and determine if relationship exists between BB test data and field test data.

6.1.3.2. Objectives

6.1.3.2.1 Objective 1 - Sample and analyze the combustion products of large-scale OB/OD operations which were conducted in a manner representing treatment site practices.

The combustion products of large-scale OB/OD operations were successfully sampled and analyzed. However, the test could not accommodate evaluation of emission product accumulation at a single site resulting from repeated detonations.

6.1.3.2.2 Objective 2 - Sample and analyze the combustion products produced by large-scale OB/OD operations which were conducted from suspended detonations.

Large-scale OD suspended detonations were successfully conducted, and the resulting clouds sampled and analyzed. While emission products were essentially the same as for non-suspended surface detonations, a more efficient conversion of the explosive carbon into CO₂ and decreased levels of the other carbon compounds were detected.

6.1.3.2.3 Objective 3 - Determine if the field test detonation data can be related to the BB test detonation data.

The initial comparison between the BB and field test data reveals that a relationship between BB and field test data can be established. The pattern that emerges is: (1) small-scale detonations in the BB test produced a more efficient conversion of TNT carbon to CO₂ than did large-scale detonations in the field; (2) the VOC levels experienced during large-scale field testing were higher than those experienced during BB testing; and (3) the semivolatile organic compounds detected and quantified were very similar.

6.1.3.2.4 Objective 4 - Provide the foundation for establishing a database on TNT and selected propellant combustion products.

The initial combustion product database for bulk TNT and selected propellant manufacturing residues was established. A list of analytes and their concentration per mass for air emissions, soil, and residue has been established.

6.1.4. Field Test Phase C

6.1.4.1. Purpose

Supplement the basic TNT and propellant data, and expand the database to include additional explosives and propellants.

6.1.4.2. Objectives

6.1.4.2.1 Objective 1 - Conduct additional TNT detonations to facilitate relating BB test results to field test results.

The additional successful TNT OD conducted during phase C added to the database of air EF's from field test phases A and B. The conclusions are discussed in paragraph 6.1.4.2.3.

6.1.4.2.2 Objective 2 - Conduct additional TNT tests to establish the reproducibility (between test precision) of TNT OD emissions.

The surface TNT tests phases A, B, and C were very reproducible, e.g., EF's for CO₂ varied from 1.26 to 1.29, CO varied from 42×10^{-3} to 61×10^{-3} , and methane varied from 1.2×10^{-3} to 1.5×10^{-3} . Section 4 contains specific results for all the compounds targeted in the OB/OD testing.

6.1.4.2.3 Objectives 3-7 - Sample and analyze the explosive and burning decomposition products of composition B, explosive D, RDX, M1 and M6 propellants, and additional propellant manufacturing residues.

a. The explosives tested during phase C produced results (emissions and levels) very similar to those results obtained for TNT tested in phases A and B. The small-scale BB test showed more efficient conversion of TNT carbon to CO₂ than found during field testing; (2) the VOC levels increased in the large-scale field test, and the semivolatile organic compounds detected and quantified during all tests were very similar.

b. The soil data from phases B and C were very similar (overlapping ranges of the concentration values), therefore all the analysis were performed on the total data package of phases B and C. Phase A was not considered because it was an ORI.

c. The propellant data was very efficient in conversion of carbon to CO₂, however the residue in the pan after burning was tested and showed the presence of 2,4-DNT, which is one of the parent compounds in the M1 and M6 propellants.

d. This phase of the study did not include analysis for metals and non-metals (elementals).

6.2. General Overall Test Program

6.2.1. Purpose

Supply waste characterization data for OB/OD permit applications under RCRA subpart X.

6.2.2. Objectives and Responses

6.2.2.1. Objective 1 - Identify and validate sampling and analytical technology, instrumentation, and procedures needed to provide RCRA subpart X data characterization.

6.2.2.1.1 The results of this phase of the OB/OD thermal-treatment emission study authenticate the innovative technologies and methodologies selected for identifying and characterizing emission products.

6.2.2.1.2 The comparable TNT data from the BB and field tests indicates that the time and costs of characterizing emissions from specific PEP materials in the inventory can be significantly reduced by using properly designed BangBox-like chambers.

6.2.2.1.3 If the comparable results, established during this test remains consistent during further BB testing, the techniques and methods developed will assist in the identification of PEP materials for which OB/OD thermal treatment methods is not applicable and for which alternative

technologies must be developed. With this knowledge, the development of alternative technologies can be focused and more cost-effective.

6.2.2.2. Objective 2 - Identify and quantify emissions and residues produced by OB/OD thermal treatment methods.

6.2.2.2.1 Identification and quantification of emission products and residues produced by OB/OD methods was accomplished for those items tested and the amount of pollutants released into the atmosphere and soil were considered inconsequential. This data was used to authenticate methodology and technology used during this phase of the study.

6.2.2.2.2 This objective will be completed during the next phase of the overall program when item- and site-specific testing will be undertaken.

6.2.2.3. Objective 3 - Provide input for development and validation of an OB/OD dispersion model.

6.2.2.3.1 An OB/OD dispersion model was developed during this phase of the study. The model will require field validation before being made available.

6.2.2.3.2 A dispersion model acceptable to EPA is an essential adjunct to the BB emission characterization data in that it provides the mechanism to generate the downwind concentration receptor locations as inputs required for support of site-specific permit applications.

6.2.2.3.3 The data obtained from sample analysis, as applied to the DPG-RTVSM model, indicates exceptionally low downwind peak and average concentrations for all pollutant categories following downwind dispersion of the detonation cloud.

6.2.2.4. Objective 4 - Identify specific items that can be treated by OB/OD thermal treatment methods without adverse environmental impact.

6.2.2.4.1 The study suggests that the bulk explosives and propellants examined during field testing will produce and release acceptable levels of emittants to the environment by surface OB/OD methods. While these results are encouraging, site-specific testing is needed to provide data to support risk assessments. Only after these risk assessments are completed may a definitive statement be made concerning the effect (if any) OB/OD operations have on human health and the environment.

6.2.2.4.2 For many items, OB/OD thermal treatment operations may be an environmentally safe means of treatment, in addition to being cost-effective. If this proves true, OB/OD should be considered for use as an integral part of a balanced DoD total demilitarization/treatment program.

6.3. Air Emissions

6.3.1. Detonation/Combustion Efficiency

A high degree of carbon conversion to CO₂ occurred for all types of PEP materials examined in this test series.

6.3.1.1. Propellants

All tested propellants consistently showed carbon conversion efficiencies exceeding 99 percent.

This is primarily a result of two factors: (1) The oxygen balance of most of the propellant materials tested was relatively high, and the propellant molecule carried most of the oxygen required for complete combustion; (2) Propellant materials were in steel pans eliminating interaction with adjacent soil. The absence of soil in the flame zone resulted in high flame temperatures and facilitated complete combustion of carbon.

6.3.1.2. Explosives

Carbon conversion efficiencies for the bulk explosive materials tested were lower than those observed for propellants, but were still in excess of 92 percent for all explosive types and configurations tested.

6.3.1.2.1 This observation applies to TNT which has a very low (-73.9 percent) oxygen balance and represents a worst case explosive from the perspective of pollutant emissions.

6.3.1.2.2 The carbon conversion efficiencies in excess of 92 percent found for low oxygen-balance surface-detonated TNT reveals that a mechanism of secondary combustion is in effect during these detonations.

a. Entrainment of ambient oxygen into the fireball region following detonation of the explosive accounts for this secondary combustion of intermediate detonation products to CO_2 .

b. Suspended detonations of TNT (for which soils is a relative unimportant consideration) produced higher carbon conversion efficiencies. This suggest the presence of soil in the immediate vicinity of the detonation (typical of surface detonations), restricts the flow of ambient air into the fireball region.

6.3.1.2.3 The carbon conversion efficiencies for other bulk-explosive types examined in this series (i.e., RDX, explosive D, composition B) show that carbon conversion efficiencies are approximately the same as for TNT, even though all of the explosives tested have higher oxygen balances than TNT.

6.3.1.2.4 The data indicates that while the oxygen balance of the explosive molecule is important, it is not the only parameter determining the degree of efficiency of the detonation.

6.3.1.2.5 All explosives have the capability to produce high-carbon-efficiency detonations if sufficient ambient oxygen is entrained following formation of the fireball.

6.3.1.2.6 The configuration of the detonation (surface vs. suspended) appears also to be an important parameter in determination of the carbon conversion efficiency.

6.3.2. Carbon Distribution

6.3.2.1. Carbon not converted to CO_2 is found in other species produced by the combustion such as carbon monoxide, methane, nonmethane hydrocarbons, organic carbon particulate and elemental carbon particulate.

6.3.2.2. In general, each of these categories, with the exception of CO_2 and CO, receives between 0.1 and 1 percent of the total original carbon.

6.3.2.3. The amount of CO formed ranged from 0.5 percent for suspended detonations to 5 percent for surface detonations.

6.3.2.4. Distribution of carbon within the nonmethane hydrocarbon category reveals a relatively high distribution of the carbon to the light, non toxic, nonmethane hydrocarbons, such as ethane, propane, acetylene, etc.

6.3.2.4.1 There is little experimental evidence to suggest that any significant portion of the source carbon goes to the heavier aromatic volatiles, such as benzene and toluene.

6.3.2.5. The elemental carbon (soot) and the organic particulate carbon categories each typically receive on the order of 0.1 to 1 percent of the carbon.

6.3.2.5.1 The amount of particulate organic carbon from soil debris in the cloud and that produced by the detonations could not be separated.

6.3.2.6. Analysis of the particulate organic material collected in these detonation and propellant cloud samples reveals that a considerable fraction is due to the environmentally ubiquitous phthalates, which were also found in the background samples.

6.3.3. Scaling Issues

6.3.3.1. The degree to which the size of the detonation affects relative distribution of pollutants released from the detonation is an important part of this study.

6.3.3.1.1 A comparison of emission factors for the various pollutant species examined in the BangBox and in the field tests shows that emission factors for potentially toxic emissions are relatively constant, despite a near 4,000-fold increase in the scale of the detonation.

6.3.3.1.2 Light gases such as CO and methane show the greatest variation in EF with changes in size of the detonation.

6.3.3.1.3 The other pollutant categories such as NO_x, VOC, and semivolatile categories show less pronounced changes in EF with changes in size of the detonation.

6.3.3.2. These results strongly indicate that BB-type testing can be successfully used to assess pollutant emissions from various explosive types and configurations.

6.3.3.3. Use of such testing will significantly reduce both the time and costs required for emission characterization of PEP materials in the DoD inventory.

6.3.4. Source Pollutant Dispersion Modeling

6.3.4.1. Results of the DPG real-time volume source dispersion model (RTVSM) for estimating ground-level concentrations of analytes from a 1-metric-ton (1000-kg) surface detonation show exceptionally low downwind peak and average concentrations for all pollutant categories following downwind dispersion of the detonation cloud.

6.3.4.2. Surface-detonation TNT events which were conducted to obtain typical EF such as CO (EF = 5×10^{-2}), benzene (EF = 1×10^{-4}) and benzo[a]pyrene (EF = 0.1×10^{-6}) reveal that ground level peak and 15-min average concentrations would be indistinguishable from background levels of these various pollutants.

6.4. Soil Deposition of OB/OD Emissions

6.4.1. OD Emissions

6.4.1.1. Total amounts of emission products for semivolatile organics can also be quantified from the mass of disturbed soil (estimated from the crater dimensions) and the concentration of analytes in the soil. For example, this method shows that 3.7 g of 2,4-dinitrotoluene will be produced and released to the soil following a 907-kg TNT detonation.

6.4.1.2. Emission products of semivolatile organics can be identified and quantified from the fallout soil at specific distances from the explosive source. This method shows that 76 mg (2 percent) of the total 3.7 g of 2,4-dinitrotoluene produced was recovered within 225 m of the detonation site.

6.4.1.3. The major portion of all the semivolatile organic particulate remains in the loose soil of the crater and ejecta area (the immediate vicinity of the crater). The loose soil is subjectively estimated to account for about 97 to 98 percent of all the semivolatiles produced.

6.4.2. OB Emissions

6.4.2.1. Open burning is very effective in volatilizing and burning the parent material. The small quantities of residue left are largely composed of char or elemental carbon.

6.4.2.2. The OB of M1 and M6 propellant resulted in a residue fraction of approximately 0.1 percent of the original mass of propellant. The 2,4-dinitrotoluene, which makes up 10 percent of the parent propellant, is reduced to 0.0025 and 0.013 percent of the residue for M1 and M6 respectively. An even greater reduction occurs in the fallout material, where the maximum 2,4-dinitrotoluene amount was 0.00009 and 0.0004 percent for M1 and M6 propellant respectively, indicating that carbon conversion is still occurring in the plume from the burning propellant.

6.4.2.3. Residue in the burn pan following the Phase C manufacturing residue burn was approximately 0.03 percent of the original mass. Using the maximum measured 2,4-dinitrotoluene

concentration of 24 ng/m² as representative of the terrain deposition from a 2-metric ton burn, results in a total deposition of 0.024 mg of 2,4-dinitrotoluene spread over 1000 m².

6.4.2.4. The OB of M30 triple base propellant burned during Phase A trials was composed of 28.0 percent nitrocellulose, 22.5 percent nitroglycerin, and 47.7 percent nitroguanidine, respectively, by weight of the parent propellant. After burning, nitroglycerin and nitroguanidine were detected and represents 0.00007 and 0.00008 percent of the residue respectively. These low residue fractions show near complete combustion of the propellant.

SECTION 7. RECOMMENDATIONS

7.1. Multiple Continuous Detonations

Conduct OD tests to determine the environmental impact to the crater area and surrounding fallout area resulting from continuous detonations at a single detonation point. This type detonation procedure is typical of those used during many treatment operations. Data on emission product accumulation in the soil is essential for evaluation of potential short- and long-term contamination. This includes subjecting the soils to Toxicity Characteristic Leaching Procedures (TCLP) to obtain critical data for the site specific characterization studies.

7.2. Buried Detonations

Conduct open detonations tests to determine the environmental impact to the air and terrain resulting from conducting buried OD. Because some treatment operations are conducted in areas which mandate that all detonations are to be buried detonations, this type of test data will be necessary to support permitting. Results of buried detonation tests will also be compared with those of surface detonation tests for an evaluation of these two methods of treatment.

7.3. Soil Extraction and Analysis

Evaluate other types of extraction and analysis programs (e.g. HPLC) in addition to refinement of GC/MS and SFC/MS, to permit rapid analysis of a large number of samples.

7.4. BangBox Design and Construction

7.4.1. Design and construct a BB to handle all typical explosive ordnance configurations (e.g. shells, mines, bombs), with a soil component using concepts and needs that have been established by the current phase of the OB/OD study. This facility will provide the means of developing a comprehensive database for selected families of PEP items.

7.4.2. Conduct OB and OD studies of those propellants and explosives used in field test phase C. The recommended testing will provide data for comparison to the large scale field tests and is necessary to establish that small scale tests will characterize emission products and confirm that large scale field tests are not necessary. The relationship between BB and field testing has been proven for TNT, but must also be established for other explosives before a generic statement can be made.

7.5. Models

7.5.1. Provide the empirical data from BB and field tests, to designated DoD personnel so that they may both verify and/or improve on existing thermodynamic equilibrium models and develop new models.

7.5.2. Complete the development and validation of the OB/OD Dispersion Model. This model is required to determine the downwind dose at receptor locations for use in risk analysis.

7.6. Technical Steering Committee

Retain the technical steering committee in its present composition to provide technical guidance on future testing. The aggregate knowledge of munitions testing (including sampling and analyses) and interpretation that is collectively possessed by the TSC, with its membership consisting of DoD, EPA, academia, USATHAMA, USAEHA, USAMC Environmental Office, and contractors, will continue to provide an invaluable interface between government agencies, academia, and industrial communities.

7.7. International Cooperation

Expand upon existing relationships between the OB/OD study program and friendly foreign government agencies investigating environmental consequences of OB/OD operations. The German Ministry of Defense has recommended that we continue these relationships, and has also requested a copy of the current OB/OD report. Contacts established with foreign agencies through

official channels offer considerable potential for expanding the U.S. database on PEP combustion products and enhancement of our technology.

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APPENDIX A - FILTER SYSTEM FLOW MEASUREMENTS

Accurate determination of particle concentration requires an accurate measurement of the volume of air sampled. Because of the varying air densities encountered during OB/OD tests, clearly defined standard reporting conditions must be established and the methods for converting from actual to standard conditions must be understood. All air volumes reported in this study are based on continuously measured flow rates and sampling durations.

The flow rate on the centerline of the transport tube was continuously monitored with a Pitot tube. As noted in the previous section, the flow in the tube is highly turbulent (Reynolds number greater than 50,000), and it is reasonable to assume that the average linear velocity down the tube and the centerline velocity are the same. The basic relationship between the velocity and the velocity pressure measured with the Pitot tube is given in equation A.1 below.

Equation A.1 Pitot Tube Velocity and Pressure.

$$V = 1096 \left(\frac{VP}{0.075 \cdot F} \right)^{0.5}$$

where V is the actual velocity in feet per minute and VP is the velocity pressure in inches of water. The 1096 term is a factor derived from the Bernoulli equation using the acceleration due to gravity, the relative densities of the manometer fluid (water) and air, and units of measurement conversions. The 0.075 term represents the density of air at standard conditions in pounds per cubic foot and F is a density correction factor to allow for differences between actual and standard conditions as given by equation A.2 below.

Equation A.2 Density Correction Factor.

$$F = \left(\frac{Press_{ambient}(mmHg)}{760} \right) \left(\frac{298}{273.1 + Temp_{ambient}(^{\circ}C)} \right)$$

Air velocity through the probe and transport tube is sufficiently fast enough that there is little change in air temperature at the Pitot tube from that measured outside the aircraft. Consequently, the externally measured ambient temperature is used for all density-correction calculations. Similarly, the static pressure regain in the transport tube is too small (a few cm of water) to significantly alter the ambient pressure from that measured by the pressure altitude sensor; therefore, the externally measured ambient pressure is used in the calculations as well. The tube velocity at ambient conditions, the density correction factor, and the tube cross-sectional area (71.26 cm²) are multiplied together to obtain the volumetric flow rate at standard conditions. After combining all the factors and the conversion factors between different systems of units, the final equation is given by equation A.3 below.

Equation A.3 Volumetric Flow rate.

$$Q = 90.71 \left(VP \cdot \frac{PRESS_{amb} (mmHg)}{273.1 + TEMP_{amb} (^{\circ}C)} \right)^{0.5}$$

where Q is the volumetric flow rate through all three filters in standard liters per second. Typical flow rates encountered with three quartz filters under normal (50 m s⁻¹) flight velocity is about 100 L s⁻¹. The factor 90.71 is a composite of the Bernoulli equation constant (1096), the cross-sectional area of the transport tube, and units of measurement conversions.

APPENDIX B - SOIL AND FALLOUT SEMIVOLATILE ORGANIC DATA

This appendix contains an example of the soil and fallout data that are on file for the OB/OD Phases A, B, and C tests. One page of the data are given in Table B.1, taken from the Phase B soil sampling and fallout data. The data sheet includes a brief description of the source of the sample, a QA custody number (which permits tracking of the sample), the sample size (in grams) on which the laboratory assay was based, and the actual laboratory results (ng/sample). These inputs were used to compute the concentrations in $\mu\text{g}/\text{kg}$ (equivalent to ppb) and ng/m^2 . In computing the concentration per square meter (ng/m^2) the total weight of sample collected and the number of square meters sampled were used. The weights shown for background, ejecta, and core samples were corrected for moisture content.

All computations were accomplished in Lotus 123®, version 2.2. The complete set of data may be requested from AMCCOM.

Table B.1 OB/OD Phase B Soil Sample Data.

Sample Source	QA Custody Number	Sample Size (g)	Compound														
			2,4-DNT	2,6-DNT	2,4,6-DNT	TNT	2-NN	N-NSDPA	1,3,5-TNB	2-NDPA	1-NP	Naph	B[a]A	B[a]P	Pyrene	Phenol	DBF
TNT-Trial-1-Ejecta																	
Site 2 Outside 1m	02873	402.1															
ng/sample			3200	BD*	39000	BD	27	6500	BD	BD	BD	1200	BD	BD	150	BD	140
µg/kg			7.96	BD	97.0	BD	0.0671	16.2	BD	BD	BD	2.98	BD	BD	0.373	BD	0.348
TNT-Trial-1-Ejecta																	
Site 2 Outside 4m	02874	280.7															
ng/sample			BD	BD	3500	BD	BD	BD	BD	BD	BD	58000	3000	BD	15000	BD	5100
µg/kg			BD	BD	12.47	BD	BD	BD	BD	BD	BD	206.7	10.68	BD	53.4	BD	18.2
TNT-Trial-1-Ejecta																	
Site 6	02945	897.5															
ng/sample			2000	70	320000	18	1000	35000	BD	BD	BD	15000	500	BD	1100	BD	200
µg/kg			2.23	0.08	357	0.02	1.11	38.9	BD	BD	BD	16.7	0.557	BD	1.23	BD	0.222
TNT-Trial-1-Fallout																	
Site 2-50m Composite	02897	202															
ng/sample			6500	440	9100	BD	14	31	BD	BD	BD	15000	1300	BD	7300	BD	120
µg/kg			32.2	2.18	45.1	BD	0.0694	0.154	BD	BD	BD	74.4	6.44	BD	36.2	BD	0.595
ng/m²			376	254	5259	BD	8.09	17.9	BD	BD	BD	8669	751	BD	4219	BD	69.4
TNT-Trial-1-Fallout																	
Sit 2-100m Composite	02898	14.1															
ng/sample			110	BD	2200	BD	BD	BD	BD	BD	BD	3100	720	BD	41	BD	410
µg/kg			7.80	BD	156	BD	BD	BD	BD	BD	BD	219	51.1	BD	2.91	BD	29.1
ng/m²			72.8	BD	1455	BD	BD	BD	BD	BD	BD	2050	476	BD	27.1	BD	271

*Below detection.

APPENDIX C - GAS SAMPLE DATA REDUCTION PROCEDURES

Introduction

The Twin Otter aircraft is used in conjunction with OB/OD tests to collect gas and particle samples from detonation or combustion clouds of various explosives and propellants. The gas sampling instruments are set up to collect and analyze gases from the aircraft air sampling tube by means of (1) direct air sampling from the tube and (2) an 80-L sampling bag that can be filled from the sampling tube during penetration of the smoke plume. Normally the gas bag is filled during several consecutive passes through the plume.

A data acquisition system (DAS) is used to acquire analog voltage signals from the gas sampling instrumentation in real-time. The gases sampled are Carbon Dioxide (TECO Model 41H); Carbon Monoxide (TECO Model 48); Oxides of Nitrogen (TECO Model 42); and Ozone (TECO Model 49). Carbon Dioxide voltages are measured at two outputs that yield an offset voltage reading (350 ppm/w background subtraction) and a direct reading voltage. Measuring both voltages allows for a measurement range that covers the range of 0 to 800 ppm CO₂. The data is stored on a "hard" disk, allowing retrieval of the raw data files and further processing, using Lotus® spreadsheets.

Each test event includes a sampling flight, a background flight and periodic span and zero checks on all instruments. Prior to each flight, zero and span data are gathered on the ground to assure proper instrument operation.

In-flight gas measurements are made from the tube until a plume pass is begun, whereupon a valve is switched to fill the teflon bag. After three passes are completed, the gases are drawn from the bag and analyzed by the various gas instruments. During analysis of the bag sample, a voltage signal to the DAS is switched "on" to mark the beginning of the measurement period and "off" to mark the end of the period. As a result, a mark is recorded in the data file to show when the instruments were sampling from the bag. At the conclusion of the sampling flight, the zeros and spans are again measured to check and allow for correction of instrument drift.

Raw Data Files

The raw data file contains all voltage outputs from the gas instruments, along with sample time and the tube/bag valve position. Zero and span average and standard-deviation values are calculated for each gas from the appropriate sampling times as recorded in the operator's notebook. A data quality check on the raw data from each instrument is carried out by graphing the voltage data as a function of time. Examination of these plots reveals when a stable reading from the bag is obtained. The graphs typically show a plateau region indicating when each instrument has stabilized on the gas concentration in the bag. The average and standard deviation values for the bag are calculated from this region. An example of the raw voltage and time data, along with the associated average voltage from the plateau region is given for the September 6, 1990 M-1 propellant burn test in Table C-1. The zero and span data are handled in a similar file not shown here for brevity.

Background Correction

Background flights are conducted to determine background readings for each gas of interest in the ambient atmosphere. Background flights are flown in the same general vicinity as the sample flights and generally on the same day. Background flights are similar to sample flights, in that zero and span data are taken before and after each flight. However, during the flight, background gas data from both the tube and the bag are taken.

Raw Gas Data Summary File

The data from the raw data file (Table C-1) are collected into one file, showing zero, span, sample, and background voltages for each gas. An example of this file for the September 6, 1990 M-1 propellant burn test is shown in Table C-2.

Gas Concentration Data File

Voltages for each gas were collected into a final spreadsheet, where the bag gas concentrations is calculated using an instrument response factor, M , by the following formula:

Equation C.1 Bag Gas Concentration Calculation.

$$M = \frac{S}{\frac{V_{si} + V_{sf}}{2} - \frac{V_{zi} + V_{zf}}{2}}$$

where

M = instrument response factor (ppm/volt)

S = span gas value (ppmv)

V_{si} = initial span reading (volt)

V_{sf} = final span reading (volt)

V_{zi} = initial zero reading (volt)

V_{zf} = final zero reading (volt).

The final bag gas concentration is calculated from the measured sample and zero-voltage averages and the response factor, M, as given by the following expression:

Equation C.2 Final Bag Gas Concentration Calculation.

$$C = (V_{sam} - \frac{V_{zi} + V_{zf}}{2}) * M$$

where C is the bag concentration in ppm, V_{sam} is the average sample voltage from the bag, and V_{zi} and V_{zf} are as defined above.

The instrument response factor, M, is calculated on a daily basis for each instrument and was entered into a final spreadsheet file, which is used to convert the voltage signal from the instrument to engineering units of parts per million (ppmv). An example of this file is given in Table C-3 for the September 6, 1990 M-1 propellant burn. All daily calibration data, including the span gas cylinder values in ppmv (column 2), the bag sample voltage (column 3) the initial and final zero voltage for each gas, columns 4 and 5, and the initial and final span voltages (columns 6 and 7) are included in the file. The initial and final zero and span voltages are averaged (columns 8 and 9) and are used to calculate an instrument response factor M, (column 10). The response factor is

multiplied by the difference between the average sample voltage (column 3) and the average zero voltage (column 8) to yield the gas concentration in ppmv (column 11). An example of this file is given in Table C-3. The final column in this table shows the gas concentration in units of ppm for each sample collected.

Finally, the background-corrected gas concentration used in all emission factor calculations is determined by subtracting the sample value from the background value for each gas of interest.

Table C-1 Example of Voltage Data from Gas Instruments During Sampling from Bag Filled During M-1 Propellant Burn, Mon, 6 Sep 90.

Time HH:MM:SS	Valve Position 0=Tube 2=Bag	CO ₂ Real volts	CO ₂ Shift volts	CO volts	NO volts	NO ₂ volts	NO _x volts	Ozone volts
12:31:50	2.000	4.990	2.661	0.347	1.025	1.792	1.470	-0.005
12:31:55	2.000	4.985	2.666	0.522	1.030	1.797	1.489	-0.005
12:32:00	2.000	4.990	2.729	0.527	1.846	-0.127	1.763	-0.005
12:32:05	2.000	4.985	2.710	0.542	1.831	-0.107	1.777	0.000
12:32:10	2.000	4.985	2.686	0.542	1.904	0.586	2.046	0.000
For brevity, the entire data collection period is not shown								
12:35:10	2.000	5.029	2.720	0.288	1.978	0.488	2.095	0.000
12:35:15	2.000	5.020	2.710	0.337	1.978	0.449	2.114	-0.010
12:35:20	2.000	4.990	2.700	0.044	1.973	0.439	2.085	-0.005
12:35:25	2.000	4.980	2.715	0.078	1.968	0.435	2.085	0.000
12:35:30	2.000	5.010	2.715	0.225	1.968	0.444	2.085	-0.010
	Average	4.995	2.712	0.087	1.974	0.450	2.093	-0.005
	Stand Dev	0.011	0.019	0.214	0.019	0.037	0.016	0.004

Table C-2a Summary Instrument Voltage Data From All Calibrations, Test Flights, and Background Flights Conducted on 6 Sep 90.

		CO ₂ REAL volts	CO ₂ SHIFT volts	CO volts	NO volts	NO ₂ volts	NO _x volts	O ₃ volts
September 06, 1990 Pre-test zero and span summary data								
ZERO	AVG	-0.005		0.006	-0.005	-0.003	-0.006	-0.006
	STD	0.002		0.017	0.002	0.004	0.003	
SPAN CO ₂ Lo, NO _x	AVG	3.347	0.349	NA ^a	2.727	1.930	3.216	NA
	STD	0.015	0.015	NA	0.004	0.023	0.005	NA
SPAN CO ₂ Hi, CO ₂ , O ₃	AVG	4.400	1.402	3.971	NA	NA	NA	0.397
	STD	0.023	0.022	0.044	NA	NA	NA	0.004
September 06 M-1 PROPELLANT BURN #1 Bag Sample Summary Data								
12.303-12.336	AVG	4.989	2.274	0.118	1.441	0.454	1.560	-0.002
	STD	0.009	0.035	0.208	0.015	0.024	0.014	0.006
September 06 M-1 PROPELLANT BURN #2 Bag Sample Summary Data								
12.536-12.592	AVG	4.995	2.712	0.087	1.974	0.450	2.093	-0.005
	STD	0.011	0.019	0.214	0.019	0.037	0.016	0.004
September 06 M-1 PROPELLANT BURN #3 Bag Sample Summary Data								
12.742-12.821	AVG	4.963	2.121	0.071	1.377	0.445	1.488	-0.005
	STD	0.079	0.031	0.218	0.016	0.021	0.013	0.004

^aNA - Only one level of span gas used in calibration for CO, NO_x, and O₃.

Table C-2b Summary Instrument Voltage Data from All Calibrations, Test Flights, and Background Flights Conducted on 6 Sep 90.

		CO ₂ REAL volts	CO ₂ SHIFT volts	CO volts	NO volts	NO ₂ volts	NO _x volts	O ₃ volts
September 06, 1990 Post-test zero and span data								
ZERO	AVG	-0.020		0.019	-0.007	-0.013	-0.013	-0.006
	STD	0.007		0.016	0.011	0.007	0.009	0.005
SPAN CO ₂ Lo,	AVG	3.435	0.436	NA*	2.766	1.890	3.242	NA
	STD	0.019	0.021	NA	0.010	0.035	0.012	NA
SPAN	AVG	4.542	1.545	3.951	NA	NA	NA	0.399
	STD	0.019	0.018	0.034	NA	NA	NA	0.024
September 06, 1990 Background flight summary data ⁴								
BKG.	AVG	3.395	0.397	0.198	-0.007	-0.005	-0.007	0.045
	STD	0.013	0.013	0.273	0.010	0.009	0.008	0.007
BKG.	AVG	3.402	0.403	0.542	-0.004	0.001	-0.010	0.025
	STD	0.036	0.035	0.928	0.013	0.008	0.008	0.008
September 06, 1990 Post-background flight zero and span summary data								
ZERO	AVG	-0.020		0.048	-0.007	-0.019	-0.012	-0.006
	STD	0.007		0.019	0.009	0.011	0.009	0.005
SPAN	AVG	3.348	0.348	NA	2.782	1.845	3.241	NA
	STD	0.011	0.010	NA	0.011	0.013	0.013	NA
SPAN	AVG	4.390	1.389	3.956	NA	NA	NA	0.394
	STD	0.011	0.009	0.019	NA	NA	NA	0.006

*NA - Only one level of span gas used in calibration for CO, NO₂, and O₃.

Table C-3a Summary Gas Instrument Data That Includes Zero, Span, and Sample Data For M-1 Propellant Burn on 6 Sep 90.

	GAS SPAN (ppm)	V_{span}^a (volts)	V_{zi}^b (volts)	V_{zi}^c (volts)	V_{zi}^d (volts)	V_{zi}^e (volts)	V_{zi}^f (volts)	M	BAG CONC (ppm)
M-1 PROPELLANT BURN #1 9/6/90 THE CO2 SHIFTED VOLTAGE IS USED FOR THE CO2 VALUE BECAUSE THE ACTUAL VOLTAGE IS OFF-SCALE									
NO	1.098	1.441	-0.005	-0.007	2.727	2.766	-0.006	0.399	0.577
NO _x	1.383	1.560	-0.006	-0.013	3.216	3.242	-0.010	0.427	0.670
NO ₂	0.280	0.454	-0.003	-0.013	1.930	1.890	-0.008	0.146	0.093
CO	7.900	0.118	0.006	0.019	3.971	3.951	0.013	2.001	0.211
CO ₂ LOW	338.000	2.274	-0.005	-0.020	3.347	3.435	-0.013	103.704	546.933
CO ₂ HIGH	450.000				4.400	4.542			
O ₃	0.400	-0.002	-0.006	-0.006	0.397	0.399	-0.006	0.990	0.004
M-1 PROPELLANT BURN #2 9/6/90									
NO	1.098	1.974	-0.005	-0.007	2.727	2.766	-0.006	0.399	0.790
NO _x	1.383	2.093	-0.006	-0.013	3.216	3.242	-0.010	0.427	0.898
NO ₂	0.280	0.450	-0.003	-0.013	1.930	1.890	-0.008	0.146	0.108
CO	7.900	0.087	0.006	0.019	3.971	3.951	0.013	2.001	0.149
CO ₂ LOW	338.000	2.712	-0.005	-0.020	3.347	3.435	-0.013	103.704	592.356
CO ₂ HIGH	450.000				4.400	4.542			
O ₃	0.400	-0.005	-0.006	-0.006	0.397	0.399	-0.006	0.990	0.001

^aAverage sample voltage from the bag.

^bInitial zero reading.

^cFinal zero reading.

^dInitial span gas reading.

^eFinal span gas reading.

^fAverage of initial and final zero reading.

^gAverage of initial and final span gas reading.

Table C-3b Summary Gas Instrument Data That Includes Zero, Span, and Sample Data For M-1 Propellant Burn on 6 Sep 90.

	GAS SPAN (ppm)	V _{span} ^a (volts)	V _{zi} ^b (volts)	V _{zf} ^c (volts)	V _{zi} ^d (volts)	V _{zf} ^e (volts)	V _{zi} ^f (volts)	V _{zf} ^g (volts)	M	BAG CONC (ppm)
M-1 PROPELLANT BURN #3 9/6/90										
NO	1.098	1.377	-0.005	-0.007	2.727	2.766	-0.006	2.747	0.399	0.552
NO _x	1.383	1.488	-0.006	-0.013	3.216	3.242	-0.010	3.229	0.427	0.640
NO ₂	0.280	0.445	-0.003	-0.013	1.930	1.890	-0.008	1.910	0.146	0.088
CO	7.900	0.071	0.006	0.019	3.971	3.951	0.013	3.961	2.001	0.117
CO ₂ LOW	338.000	2.121	-0.005	-0.020	3.347	3.435	-0.013	3.391	103.704	531.067
CO ₂ HIGH	450.000				4.400	4.542		4.471		
O ₃	0.400	-0.005	-0.006	-0.006	0.397	0.399	-0.006	0.398	0.990	0.001
BACKGROUND FLIGHT 9/6/90 BAG SAMPLE										
NO	1.098	-0.004	-0.007	-0.007	2.766	2.782	-0.007	2.774	0.395	0.001
NO _x	1.383	-0.010	-0.013	-0.012	3.242	3.241	-0.013	3.242	0.425	0.001
NO ₂	0.280	0.001	-0.013	-0.019	1.890	1.845	-0.016	1.868	0.149	0.000
CO	7.900	0.542	0.019	0.048	3.951	3.956	0.034	3.954	2.015	1.025
CO ₂ LOW	338.000	3.402	-0.020	-0.020	3.435	3.348	-0.020	3.392	104.235	354.606
CO ₂ HIGH	450.000				4.542	4.390		4.466		
O ₃	0.400	0.025	-0.006	-0.006	0.399	0.394	-0.006	0.397	0.994	0.031

^a Average sample voltage from the bag.

^b Initial zero reading.

^c Final zero reading.

^d Initial span gas reading.

^e Final span gas reading.

^f Average of initial and final zero reading.

^g Average of initial and final span gas reading.

OBOD GAS BAG DATA FROM SEPT 6, 1990

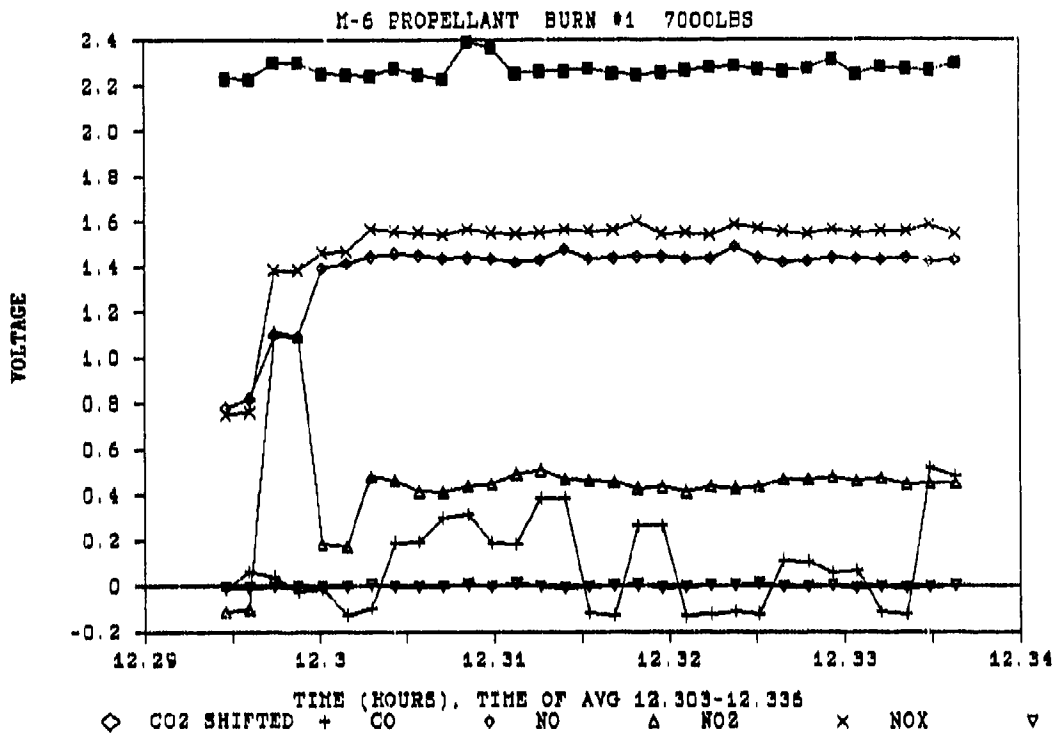


Figure C-1 Raw Voltage Data From Gas Instruments While Sampling From Bag Following The First M-1 Propellant Test.

■ valve open position voltage

OBOD GAS BAG DATA FROM SEPT 6, 1990

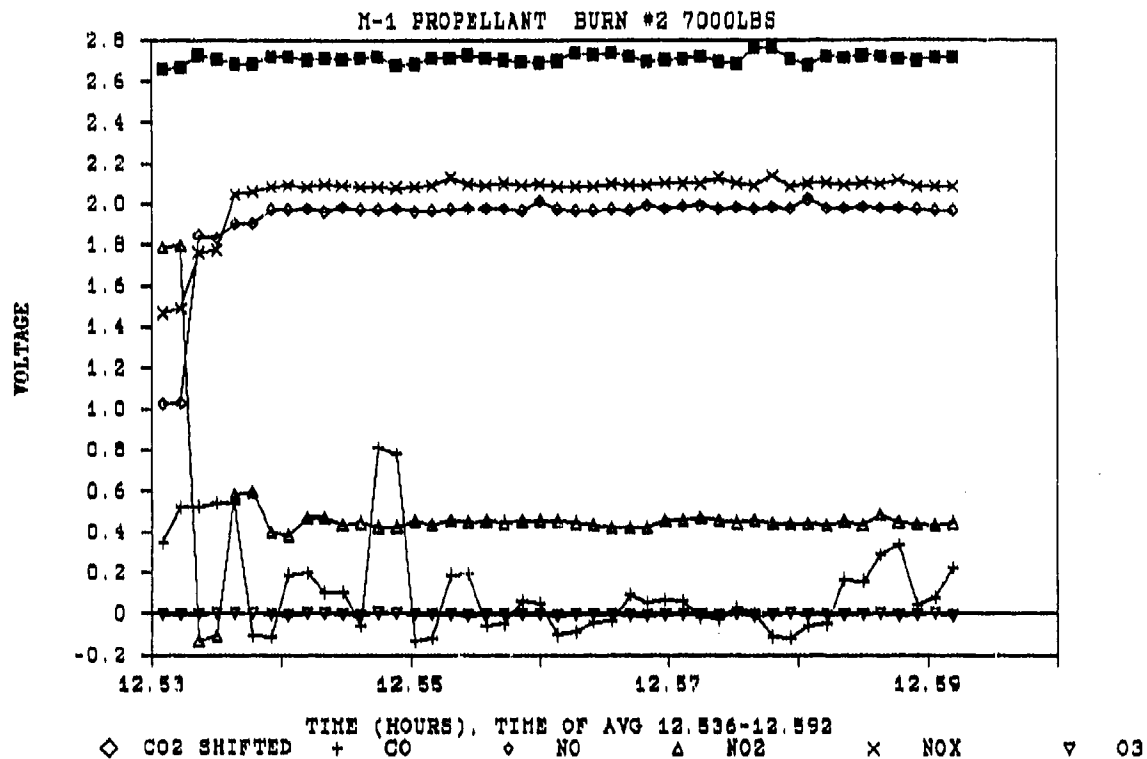


Figure C-2 Raw Voltage Data From Gas Instrument While Sampling From Bag Following Second M-1 Propellant Burn.

■ valve open position voltage

APPENDIX D - PARTICULATE MATTER DATA REDUCTION

Particulate matter data is handled in conjunction with other data to calculate average cloud particulate matter concentrations, and in the special case of propellant burns, a particulate matter emission factor. The calculation begins with the weight gain on each of the three filters used to collect the particulate sample. The weight gain is determined from a weighing of the filter prior to sampling and after sampling. Control filters are weighed along with sample filters to correct for differences in filter weight that are attributable to filter handling or storage conditions. For example, in the Phase C test, the data is contained in a worksheet named PHZCWGT.WK1 shown excerpted in Table D-1. Also included in this spreadsheet for each filter sample is a measure of the total volume of air sampled through the filter during all aircraft passes through the plume as measured by a pitot tube installed on the centerline of the transport tube. The total volume is determined by a continuous measure of the linear air velocity (as calculated from velocity pressure) through the tube whenever the filter sample port was open. An average velocity, calculated over the entire filter sampling interval and corrected for atmospheric pressure changes and temperature, is multiplied by the cross sectional area of the tube to yield the total sampled volume of air at standard conditions (25 °C and 1 atmosphere).

The average background corrected particle mass concentration, C , in the cloud as measured over multiple aircraft passes through the cloud is given by:

$$C = \frac{M_s}{V_s} - \frac{M_b}{V_b}$$

where M_s and M_b is the total particulate mass measured on the sample and background filters, and V_s and V_b is the total air volume drawn through the filter for the sample and background sample.

In the case of the propellant burns, the particle emissions are assumed to originate from the combustion process only (no entrained soil).

Table D-1 Filter Weight and Volume Data.

Date	Test Description	Adjusted Total Mass (mg)	Total Sample Volume (m ³)	Mass Conc (mg m ⁻³)
August 29	Background	3.9	226.15	0.017
August 29	M-6 Propellant #3	27.2	10.07	2.7
August 30	Background	3.1	214.48	0.014
August 30	M-6 Propellant #4	30.5	10.78	2.8
September 05	Background	2.9	223.28	0.013
September 05	M-1 Propellant #1	15.8	11.90	1.3
September 06	M-1 Propellant #2	24.6	9.58	2.6
September 06	Background	3.0	182.79	0.016
September 18	Background	7.0	193.33	0.036
September 18	Comp B #1 (3x)	2190.8	10.05	218.0
September 18	Comp B #2 (3x)	1649.7	8.66	190.5

Under these circumstances, a total particulate matter emission factor can be calculated by the following:

$$EF_{part} = \frac{C_{part}}{C_{tot}} * f_c$$

where EF_{part} is the particulate matter emission factor, C_{part} is the average cloud particulate matter concentration, C_{tot} is the background corrected total carbon content in the sampled volume, (Table D-2) and f_c is the carbon mass fraction in the original propellant material.

Table D-2 Total Background Corrected Carbon Content in Air Samples.

Date	Test Description	Background Corrected Total Carbon (mg C m ⁻³)
August 29	M-6 Propellant	176.14
August 30	M-6 Propellant	142.02
September 05	M-1 Propellant	180.05
September 06	M-1 Propellant	176.83

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APPENDIX E - VOLATILE ORGANIC COMPOUND DATA-REDUCTION

Emission factors (EF) are calculated for volatile organic compounds (VOC) using sample analysis data provided by the Oregon Graduate Institute for Science and Technology for each of the 6-L canister samples collected during aircraft sampling of detonation or combustion clouds. The emission factors are determined using the carbon balance technique that is also employed for calculation of gas and semivolatile organic EF's. The VOC analysis procedure provides concentration levels for carbon monoxide, carbon dioxide, methane as well as most hydrocarbons in the C₂ through C₁₀ range. Data are provided in tabular format for both background and test samples as shown in Tables E-1, a, b and c; and E-2 a, b, and c for an M-1 propellant test conducted on September 06, 1990 (Note: Although not shown on this particular table, CO₂ concentrations for the tube background sample and tube test sample were 348 and 670 ppm respectively. The CO₂ data is provided in another analysis report not included here for the sake of brevity.)

The EF calculation is begun by subtracting the background level of the VOC species of interest from the level determined in the test sample. This value multiplied by the carbon fraction in the original material and is then divided by the total carbon in the sample as represented by the background corrected CO and CO₂ concentration levels. Here, as in other cases, CO and CO₂ are presumed to account for over 99 percent of the total carbon released in the burn. Consequently, the small carbon contributions from methane and total non-methane hydrocarbons as well as the carbon appearing as soot are neglected for the sake of computational simplicity. Their omission results in, at worst, an error in the EF of ± 5 percent. In most instances it will be less than one percent. Emission factors were calculated for only several categories of VOC in order to consolidate the vast amount of information contained in each one of these VOC analysis sheets. Normally calculations were carried out for methane (CH₄), total non-methane hydrocarbons (TNMHC) and benzene. Benzene (as probably the most toxic compound on the list) was selected in order to have some indicator of a "toxic" VOC compound used as a general marker or indicator of overall VOC toxicity in the sample.

The expression used to calculate the EF for a particular species appearing among the products of detonation or burning, is given by the equation E.1.

Equation E.1 Emission Factor Calculation.

$$EF_x = \frac{(X_t - X_b) f_c}{([CO]_t - [CO]_b) 0.429 + ([CO_2]_t - [CO_2]_b) 0.273}$$

where

- EF_x = emission factor for the species of interest
- [X] = species concentration in the test sample
- [X]_b = species concentration in the background sample
- f_c = fraction of carbon in the original test (PEP) material (0.303 for M-1)
- [CO₂]_t = CO₂ concentration in the test sample
- [CO₂]_b = CO₂ concentration in the background sample
- [CO]_t = CO concentration in the test sample
- [CO]_b = CO concentration in the background sample

The factor 0.429 and 0.273, are the fractions of the gases, CO and CO₂, respectively which are carbon.

Note: All concentrations must be expressed in self-consistent units of whatever kind. In this report concentrations are expressed both in parts per million by volume (ppmV) and in micrograms per cubic meter of dry air at 25°C and 1 atmosphere assuming ideal gas behavior (an excellent assumption at the relatively low pressures involved).

Table E-1a Volatile Organic Compound Background Data for M-1 Propellant

Date 09/06/90 Location: OBOD		Can # SDA168 Tube Sample # 168	
CO 78, ppm CH ₄ 1778 ppm	$\mu\text{g}/\text{m}^3$	ppbv-c	Percent
Total Identified Hydrocarbons	54.2	90.5	44.7
Alkanes (Parafins)	43.0	71.8	35.3
Alkenes (Olefins)		0.0	0.0
Aromatics	11.2	18.7	9.2
Terpenes		0.0	0.0
Total Unidentified Hydrocarbons	67.0	111.9	55.3
Total Nonmethane Hydrocarbons	121.2	202.4	100.0
Compounds	$\mu\text{g}/\text{m}^3$	ppbv-c	ID code
Ethane	0.2	0.3	1
Ethylene			2
Acetylene			3
Propane	1.7	2.8	4
Propene			5
i-butane	0.5	0.8	6
i-butene			7
1-butene			8
1,3-butadiene			8a
n-butane	0.5	0.8	9
trans-2-butene			10
2,2-dimethylpropane			11
cis-2-butene			12
3-methyl-1-butene			13
i-pentane			14
1-pentene			15
2-methyl-1-butene			16
n-pentane			17
Isoprene			18
trans-2-pentene			19
cis-2-pentene			20
2-methyl-2-butene			21
2,2-dimethylbutane	0.5	0.8	22

Table E-1b Volatile Organic Compound Background Data for M-1 Propellant.

Date 09/06/90 Location: OBOD		Can # SDA168	Tube
		Sample # 168	
Compound	$\mu\text{g}/\text{m}^3$	ppbv-c	ID Code
Cyclopentene			23
4-methyl-1-pentene			24
Cyclopentane	0.5	0.8	25
2,3-dimethylbutane	0.6	1.0	26
cis-4-methyl-2-pentene			26a
2-methylpentane	3.4	5.7	27
3-methylpentane	1.8	3.0	28
2-methyl-1-pentene			29
1-hexane			30
n-hexane	4.8	8.0	31
trans-2-hexene			32
2-methyl-2-pentene			33
cis-2-hexene			35
alpha-thujene			T1
Camphene			T2
Sabinene			T3
Mercene			T4
beta-lterpinene			T4a
Sesquiterpine			T11
beta-terpinene			T5
Methylcyclopentene	1.9	3.2	36
2,4-dimethylpentane	0.3	0.5	37
Benzene	1.8	3.0	38
Cyclohexane	3.0	5.0	39
2-methylhexane	1.5	2.5	39a
2,3-dimethylhexane	0.4	0.7	40
3-methylhexane	1.9	3.2	41
n-heptane	2.3	3.8	43
methylcyclohexane	3.2	5.3	44
2,4-dimethylhexane			45
2,3,4-trimethylpentane			46

Table E-1c Volatile Organic Compound Background Data for M-1 Propellant.

Date 09/06/90 Location: OBOD		Can # SDA1168 Tube Sample # 168	
Compound	$\mu\text{g}/\text{m}^3$	ppbv-c	ID Code
Toluene	3.1	5.2	47
2,3-dimethylhexane			48
2-methylheptane	0.5	0.8	49
3-ethylhexane	0.4	0.7	50
n-octane	1.1	1.8	51
Ethylcyclohexane			52
Ethylbenzene	0.8	1.3	53
m-xylene & p-xylene	2.4	4.0	54
Styrene	1.1	1.8	56
o-xylene	0.5	0.8	57
n-nonane	1.2	2.0	58
alpha-pinene			59
i-propylbenzene			60
n-propylbenzene			61
p-ethyltoluene	0.3	0.5	62
m-ethyltoluene	0.4	0.7	63
1,3,5-trimethylbenzene			64
o-ethyltoluene			65
beta-pinene			66
Methylstyrene			67a
1,2,4-trimethylbenzene	0.8	1.3	68
n-decane	1.4	2.3	69
1,2,3-trimethylbenzene			69a
1,3-diethylbenzene			69b
1,4-diethylbenzene			69c
alpha-terpinene			T6
2-carene			T7
beta-phellandrene			T8
gamma-terpinene			T9
d-limonene			70
Terpinene			T10

Table E-2a Volatile Organic Compound Test Data for M-1 Propellant.

Date 09/06/90 Location: OBOD		Can # SDA184 Tube Sample # 184	
CO 78, ppm CH ₄ 1778 ppm	$\mu\text{g}/\text{m}^3$	ppbv-c	Percent
Total Identified Hydrocarbons	16.8	28.1	31.5
Alkanes (Parafins)	10.8	18.0	20.2
Alkenes (Olefins)	2.1	3.5	3.9
Aromatics	3.9	6.5	7.3
Terpenes		0.0	0.0
Total Unidentified Hydrocarbons	36.7	61.3	68.6
Total Nonmethane Hydrocarbons	53.5	89.3	100.1
Compounds	$\mu\text{g}/\text{m}^3$	ppbv-c	ID code
Ethane	1.3	2.2	1
Ethylene			2
Acetylene			3
Propane	0.8	1.3	4
Propene			5
i-butane			6
i-butene	1.2	2.0	7
1-butene			8
1,3-butadiene			8a
n-butane	0.6	1.0	9
trans-2-butene			10
2,2-dimethylpropane			11
cis-2-butene			12
3-methyl-1-butene			13
i-pentane			14
1-pentene			15
2-methyl-1-butene			16
n-pentane			17
Isoprene			18
trans-2-pentene			19
cis-2-pentene			20
2-methyl-2-butene			21
2,2-dimethylbutane	2.3	3.8	22

Table E-2b Volatile Organic Compound Test Data for M-1 Propellant.

Date 09/06/90 Location: OBOD		Can # SDA184 Tube Sample # 184	
Compound	$\mu\text{g}/\text{m}^3$	ppbv-c	ID Code
Cyclopentene	0.2	0.3	23
4-methyl-1-pentene	0.7		24
Cyclopentane	1.2		25
2,3-dimethylbutane			26
cis-4-methyl-2-pentene			26a
2-methylpentane			27
3-methylpentane			28
2-methyl-1-pentene			29
1-hexane			30
n-hexane	0.4	0.7	31
trans-2-hexene			32
2-methyl-2-pentene			33
cis-2-hexene			35
alpha-thujene			T1
Camphene			T2
Sabinene			T3
Mercene			T4
beta-lterpinene			T4a
Sesquiterpine			T11
beta-terpinene			T5
Methylcyclopentene	0.4	0.7	36
2,4-dimethylpentane			37
Benzene	0.3	0.5	38
Cyclohexane	0.2	0.3	39
2-methylhexane	0.5	0.8	39a
2,3-dimethylhexane			40
3-methylhexane	1.2	2.0	41
n-heptane	0.3	0.5	43
methylcyclohexane			44
2,4-dimethylhexane			45
2,3,4-trimethylpentane	0.5	0.8	46

Table E-2c Volatile Organic Compound Test Data for M-1 Propellant.

Date 09/06/90 Location: OBOD		Can # SDA184 Tube Sample # 184	
Compound	$\mu\text{g}/\text{m}^3$	ppbv-c	ID Code
Toluene	0.4	0.7	47
2,3-dimethylhexane			48
2-methylheptane			49
3-ethylhexane			50
n-octane	0.2	0.3	51
Ethylcyclohexane			52
Ethylbenzene			53
m-xylene & p-xylene			54
Styrene			56
o-xylene	1.3	2.2	57
n-nonane			58
alpha-pinene			59
l-propylbenzene			60
n-propylbenzene			61
p-ethyltoluene			62
m-ethyltoluene	0.3	0.5	63
1,3,5-trimethylbenzene			64
o-ethyltoluene			65
beta-pinene			66
Methylstyrene			67a
1,2,4-trimethylbenzene	1.6	2.7	68
n-decane	2.1	3.5	69
1,2,3-trimethylbenzene			69a
1,3-diethylbenzene			69b
1,4-diethylbenzene			69c
alpha-terpinene			T6
2-carene			T7
beta-phellandrene			T8
gamma-terpinene			T9
d-limonene			70
Terpinene			T10

APPENDIX F - SEMIVOLATILE ORGANIC DATA REDUCTION

The principles used in the calculation of the emission factors for semivolatile organic compounds are the same as used for gas and VOC analysis. Data obtained from the laboratory are reported in nanograms of a particular target analyte per total sample received, whether filters, soil, or fallout pan. If all three of the exposed air filters from a given test were analyzed, the results from all three are simply summed to obtain the total amount of a given substance collected in the test. In selected cases where only two of the three filters were analyzed (the third being used for a different analysis) it was assumed that all three collected equal amounts of material and the total adjusted accordingly.

The total amount of a given analyte from each test sample is then divided by the volume of sample air drawn through all of the filters, reduced to standard cubic meters, as measured by a Pitot tube mounted in the center line of the aerosol transport tube on the aircraft to yield its concentration in nanograms per cubic meter. (See Appendix A for procedures to calculate tube air velocity and total sample volume). Similar calculations are carried out for the background samples collected the same date and location. Each target analyte air concentration value is then used along with the total net carbon concentration measured in the sample and the carbon fraction of the PEP material being tested to calculate its respective emission factor.

A complication in the calculation results from the fact the filter samples represent the summation from sampling the emission clouds from three distinct successive detonations or burns, (This is done to acquire an adequately sized sample). whereas the required accompanying CO and CO₂ assays are obtained from an 80-L Teflon® bag attached to the same aerosol transport tube as the filters. However, a separate CO₂ and CO sample is collected for every pass through the emission cloud. A weighted average of CO₂ and CO gas concentrations is calculated using the fraction of the total air volume for all of the tests of a given type represented by a given bag sample. Assuming well mixed conditions the composition of a bag sample in a given instance should be the same as that drawn simultaneously through the filters.

The expression used to calculate the EF for the semivolatile organic target analytes is then as follows:

Equation F-1 Emission Factor Calculation for Semivolatiles.

$$EF_x = \frac{\left(\frac{M_t}{V_t} - \frac{M_b}{V_b} \right) f_c}{C_{wt}}$$

where

- EF_x = emission factor (EF) of a specified target analyte (x)
- M_t = total test analyte mass on all test filters
- V_t = total test air volume drawn through all test filters
- M_b = total background analyte mass on all background filters
- V_b = total background air volume drawn through all background filters
- f_c = carbon fraction of the test material (0.303 for M-1 propellant)
- C_{wt} = weighted average total carbon concentration in the sample

Note: All values must be expressed in consistent units.

The total weighted average carbon concentration, C_{tot} , is given by the following:

Equation F-2 Calculation of Total Weighted Average Carbon Concentration.

$$C_{tot} = \sum \left(\frac{V_i}{V_{tot}} ([\overline{CO_2}]_i + [\overline{CO}]_i) 0.491 \right)$$

where

- C_{tot} = total carbon in sample (mg m^{-3})
- V_i = total standard gas volume drawn through filters in i-th sample
- V_{tot} = total standard gas volume drawn through all filters on all samples from a given test
- $[\overline{CO_2}]_i$ = average background corrected CO_2 concentration (ppmV) in the i-th bag sample
- $[\overline{CO}]_i$ = average background corrected CO concentration (ppmV) in the i-th bag sample

Notes: The factor, 0.491 converts the ppmV concentration of any gas containing only one atom of carbon per molecule behaving ideally to mg/m^3 carbon at standard conditions.

The summation is carried out for $i = 1$ to $i = n$, where n is the total number of bag samples collected during a given filter sampling.

Table F-1 Semivolatile Target Analyte Loadings on Background and Test Filters for 6 Sep 90 M-1 Propellant Test.

Analyte	Total Sample Loading (ng)					
	Filter 3427 Bkgnd	Filter 3428 Bkgnd	Filter 3429 Bkgnd	Filter 3423 Test	Filter 3424 Test	Filter 3425 Test
2,4 Dinitrotoluene	1.1	1.0	1.2	1.1	1.0	1.5
2,6 Dinitrotoluene						
2,4,6 Trinitrotoluene						
2-Nitronaphthalene						
N-Nitrosodiphenylamine						
1,3,5-Trinitrobenzene						
2-Nitrodiphenylamine						
1-Nitropyrene						
Naphthalene	33.2				30.5	23.0
Benzo[a]anthracene						
Benzo[a]pyrene						
Pyrene						
Phenol	4.9	4.8		0.9	2.7	2.5
Dibenzofuran						
Diphenylamine		0.1		0.1		

No data entry - indicates below detection level.

Table F-2 Air Volume and Gas Concentration Data or 6 Sep 90 M-1 Propellant Test.

Parameter	Background Sample	Test Sample
Total Sample Vol. (m ³)	182.79	9.58
Test 1 Sample Vol. (m ³)		2.88
Test 2 Sample Vol. (m ³)		3.84
Test 3 Sample Vol. (m ³)		2.86
Bkgnd-corr CO ₂ / CO Bag 1 (ppm)		192 / ND
Bkgnd-corr CO ₂ / CO Bag 2 (ppm)		138 / ND
Bkgnd-corr CO ₂ / CO Bag 3 (ppm)		177 / ND

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APPENDIX G - SEMIVOLATILE ORGANIC ASSAY

The semivolatiles collected on soil particles and sampled by Teflon[®] coated glass fiber filters and soil ejecta and fallout were all assayed by SFC/MS and most samples were also assayed by GC/MS. The RDX semivolatile data is shown in this appendix as an example of the data available for each detonation or burn. RDX was chosen because two of the compounds, N-nitrosodiphenylamine and RDX are not identified and quantified with the GC/MS method of assay; however, they are identified and quantified with the SFC/MS method of assay. Table G.1 gives the QA custody number used to identify each sample from the initial field collection through the data analysis, the origin of the collected sample, and the weight of the soil that was extracted for the sample assay. Tables G.2a through G.2d show the concentration determined for each sample by the two methods of assay. Duplicate samples were collected for all the assays from sites D1, D3, and D5 (e.g. samples number 4065 and 4069 are independent background samples).

Table G.1 Sample Identification and Weight of Particles in Sample.

QA CUSTODY NUMBER	LOCATION	SAMPLE TYPE	SAMPLE SOURCE	WEIGHT OF SAMPLE (g)
3613	Aircraft	Filter	Air (Trial 1)	
3614	Aircraft	Filter	Air (Background)	
3615	Aircraft	Filter	Air (Trial 2)	
4065	Site D1, D3, D5	Background	Detonation site	372.8
4069	Site D1, D3, D5	Background	Detonation site	372.2
4067	Site D2, D4, D6	Background	Detonation site	377.8
4634	Site D1, D3, D5	Ejecta	Detonation crater	375.9
4640	Site D1, D3, D5	Ejecta	Detonation crater	359.1
4646	Site D2, D4, D6	Ejecta	Detonation crater	386.6
4622	Site D1, D3, D5	Fallout	50m from detonation	369.8
4623	Site D1, D3, D5	Fallout	50m from detonation	396.1
4624	Site D1, D3, D5	Fallout	100m from detonation	236.2
4625	Site D1, D3, D5	Fallout	100m from detonation	102.4
4626	Site D1, D3, D5	Fallout	150m from detonation	22.8
4627	Site D1, D3, D5	Fallout	150m from detonation	2.57
4628	Site D1, D3, D5	Fallout	200m from detonation	26.3
4629	Site D1, D3, D5	Fallout	200m from detonation	1.02
4648	Site D2, D4, D6	Fallout	50m from detonation	356.3
4649	Site D2, D4, D6	Fallout	100m from detonation	268.4
4650	Site D2, D4, D6	Fallout	150m from detonation	13.4
4651	Site D2, D4, D6	Fallout	200m from detonation	2.41

Table G-2a Data of the Supercritical-Fluid Chromatography/Mass Spectrometry and Gas Chromatography/Mass Spectrometry for the RDX Detonations.

SEMIVOLATILE COMPOUNDS	3613		3614		3615		4065		4069		4067	
	SFC/MS (ng/MI)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)
2,4-Dinitrotoluene	410	230	220	210	240	330	220	500	270	920	210	410
2,6-Dinitrotoluene	33	18	160	33	73	20	120	69	75	41	21	28
2,4,6-Trinitrotoluene	61	18	260	BD ^a	160	BD	240	71	220	65	61	BD
2-Nitronaphthalene	85	BD	350	BD	91	BD	190	45	120	31	68	26
N-Nitrosodiphenylamine	BD	NA ^b	BD	NA	BD	NA	BD	NA	BD	NA	BD	NA
1,3,5-Trinitrobenzene	92	BD	190	BD	48	BD	110	1	51	2	71	35
2-Nitrodiphenylamine	60	BD	180	BD	60	BD	110	400	80	430	44	230
1-Nitropyrene	66	BD	150	BD	83	BD	300	BD	170	BD	74	BD
RDX	2200	NA	4600	NA	3400	NA	1400	NA	1100	NA	400	NA
Naphthalene	330	1600	210	970	310	1900	120	81	170	160	41	140
Benz[a]anthracene	96	190	91	BD	65	BD	66	91	68	BD	63	56
Benzo[a]pyrene	270	BD	76	BD	41	BD	53	BD	61	BD	55	BD
Pyrene	180	380	260	410	320	500	1	28	23	17	14	27
Phenol	— ^c	—	—	—	—	—	—	—	—	—	—	—
Dibenzofuran	150	140	110	53	3000	120	30	33	18	48	BD	51
Diphenylamine	45	64	250	43	150	38	91	7	92	12	95	11

^aBD - below detection limit.

^bNA - a target analyte not detected by GC/MS.

^cPhenol was lost in the extraction of the semivolatiles.

Table G.2b Data of the Supercritical-Fluid Chromatography/Mass Spectrometry and Gas Chromatography/Mass Spectrometry for the RDX Detonations.

SEMIVOLATILE COMPOUNDS	4634		4640		4646		4622		4623		4624	
	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)
2,4-Dinitrotoluene	740	660	340	440	130	220	320	110	120	170	110	18
2,6-Dinitrotoluene	340	100	93	35	31	1	310	7	100	BD*	87	BD
2,4,6-Trinitrotoluene	250	77	100	56	110	16	530	270	2000	1600	1000	42
2-Nitronaphthalene	340	71	110	35	50	7	580	49	220	BD	79	BD
N-Nitrosodiphenylamine	650	NA ^b	590	NA	230	NA	1400	NA	BD	NA	BD	NA
1,3,5-Trinitrobenzene	290	130	47	420	79	BD	340	BD	58	BD	66	BD
2-Nitrodiphenylamine	73	BD	49	BD	66	18	240	240	220	BD	120	BD
1-Nitropyrene	BD	BD	83	BD	18	52	370	BD	40	BD	80	BD
RDX	4600	NA	5300	NA	1900	NA	4000	NA	18000	NA	6800	NA
Naphthalene	2000	2600	1900	2000	1200	2000	530	210	420	260	210	87
Benz[a]anthracene	910	520	750	740	680	210	4300	1100	4000	1000	BD	130
Benzo[a]pyrene	BD	BD	97	BD	160	210	BD	BD	1160	BD	120	BD
Pyrene	200	120	1900	1700	1200	20	1000	700	1600	2100	600	190
Phenol	— ^c	—	—	—	—	—	—	—	—	—	—	—
Dibenzofuran	260	170	340	390	340	290	130	77	BD	180	BD	27
Diphenylamine	180	150	160	100	BD	2	BD	19	BD	63	BD	3

*BD - below detection limit.

^bNA - a target analyte not detected by GC/MS.

^cPhenol was lost in the extraction of the semivolatile.

Table G-2c Data of the Supercritical-Fluid Chromatography/Mass Spectrometry and Gas Chromatography/Mass Spectrometry for the RDX Detonations.

SEMIVOLATILE COMPOUNDS	4625			4626			4627			4628			4629			4648		
	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	
2,4-Dinitrotoluene	81	110	49	150		280	140	290	410	270	270	730	1300					
2,6-Dinitrotoluene	70	BD*	34	BD		340	40	15	100	BD	19	29	170					
2,4,6-Trinitrotoluene	490	77	280	BD		390	60	63	160	20	40	340	480					
2-Nitronaphthalene	110	14	88	17		300	78	59	170	22	28	130	410					
N-Nitrosodiphenylamine	430	NA*	440	NA		550	NA	NA	690	170	NA	370	NA					
1,3,5-Trinitrobenzene	26	BD	18	BD		510	BD	41	210	6	11	33	BD					
2-Nitrodiphenylamine	120	BD	120	BD		200	BD	BD	130	29	140	250	BD					
1-Nitropyrene	150	BD	130	BD		310	BD	130	300	8	BD	16	BD					
RDX	13000	NA	16000	NA		3700	NA	NA	29000	1000	NA	11000	NA					
Naphthalene	180	82	740	BD		550	170	1800	250	750	220	450	2200					
Benz[a]anthracene	900	180	37	37		560	BD	110	800	61	80	640	420					
Benzo[a]pyrene	100	BD	74	90		420	BD	BD	BD	BD	BD	680	BD					
Pyrene	580	320	280	110		640	BD	200	920	230	72	1900	2600					
Phenol	— ^c	—	—	—		—	—	—	—	—	—	—	—					
Dibenzofuran	320	250	BD	63		240	110	200	BD	35	31	BD	290					
Diphenylamine	BD	12	BD	25		220	50	380	480	26	35	240	520					

^aBD - below detection limit.

^bNA - a target analyte not detected by GC/MS.

^cPhenol was lost in the extraction of the semivolatile.

Table G.2d Data of the Supercritical-Fluid Chromatography/Mass Spectrometry and Gas Chromatography/Mass Spectrometry for the RDX Detonations.

SEMIVOLATILE COMPOUNDS	4649		4650		4651	
	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)	SFC/MS (ng/mL)	GC/MS (ng/mL)
2,4-Dinitrotoluene	43	59	500	90	230	230
2,6-Dinitrotoluene	4	9	11	29	160	BD ^a
2,4,6-Trinitrotoluene	130	BD	1700	54	230	23
2-Nitronaphthalene	170	20	BD	50	350	8
N-Nitrosodiphenylamine	9	NA ^b	88	NA	35	NA
1,3,5-Trinitrobenzene	2	52	14	BD	230	BD
2-Nitrodiphenylamine	19	60	BD	42	84	33
1-Nitropyrene	BD	BD	BD	BD	170	BD
RDX	2300	NA	BD	NA	690	NA
Naphthalene	220	160	200	76	100	BD
Benz[a]anthracene	49	76	BD	BD	85	BD
Benzo[a]pyrene	6	BD	34	BD	190	BD
Pyrene	1	35	120	BD	100	43
Phenol	---	---	---	---	---	---
Dibenzofuran	BD	99	150	140	110	64
Diphenylamine	BD	46	BD	140	110	10

^aBD - below detection limit.

^bNA - a target analyte not detected by GC/MS.

^cPhenol was lost in the extraction of the semivolatile.

APPENDIX H - REFERENCES

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APPENDIX I - ABBREVIATIONS

ACGIH	American Conference of Governmental Industrial Hygienists
AEHA	U.S. Army Environmental Hygiene Agency, Aberdeen Proving Ground, Maryland
AFB	Air Force Base
AMC	U.S. Army Materiel Command, Alexandria, Virginia
AMCCOM	U.S. Army Armament, Munitions and Chemical Command, Rock Island, Illinois
amino-PAH	aminopolycyclic aromatic hydrocarbons
ANOVA	analysis of variance
AP	ammonium perchlorate
APS	aerodynamic particle sizer
ASASP	active scattering aerosol spectrometer probe
AWL	Alpine West Laboratories, Provo, Utah
BB	BangBox
BCD	Battelle Columbus Division, Columbus, Ohio
BD	target analyte not found in concentrations above detection limits
BYU	Brigham Young University, Provo, Utah
CAA	Clean Air Act
CDD	chlorinated dibenzodioxin
CDF	chlorinated dibenzofuran
CI-SIM	chemical ionization, selective-ion monitoring
CSI	Columbia Scientific Instruments
C·V	concentration times cloud volume method
CWA	Clean Water Act
DMC	Data Management Center
DMPS	differential mobility particle sizer
DoD	Department of Defense
DPG	U.S. Army Dugway Proving Ground, Dugway, Utah
EC	electron capture <i>or</i> elemental carbon
ECD	electron capture detector
EDAX	energy-dispersive X-ray analysis
EER	Energy and Environmental Research Corporation, Irvine, California

EF	emission factor(s)
EI	electron impact
EI-MS	mass spectrometer used in the electron impact ionization mode
EI/MS	electron impact ionization/ mass spectrometry
EIS	environmental impact statement
ELI	Environmental Labs, Incorporated, Provo, Utah
EOD	explosive ordnance disposal
EPA	U.S. Environmental Protection Agency
EPO	Environmental Protection Office, U.S. Army Dugway Proving Ground, Dugway, Utah
ER	expansion ratio
FID	flame ionization detector
FSSP	forward scattering spectrometer probe
FTIR	Fourier Transform Infrared Spectrometry
FWAC	fixed-wing aircraft
GC	gas chromatograph(y)
GC-ECD	gas chromatography with an electron capture detector
GC-FID	gas chromatography with a flame ionization detector
GC/MS	gas chromatography-mass spectrometry
GLP	good laboratory practices
HE	high explosive
HMX	octamethylenehexanitramine
HNBB	hexanitrobibenzyl
HRGC/HRMS	combined capillary column gas chromatography/high resolution mass spectrometry
HS	high-speed
LASD	Los Angeles Sheriff Department
LBL	Lawrence Berkeley Laboratory, Berkeley, California
LC	liquid chromatography
LOD	limit of detection
LOI	letter(s) of instruction

MR	multiple range
MRI	Midwest Research Institute, Kansas City, Kansas
MS	mass spectrometry (or mass spectrometer)
MSA	Mine Safety and Appliance Company
NA	not targeted for analysis <i>or</i> not applicable
NASA	National Aeronautical and Space Administration
NATICH	National Air Toxics Information Clearinghouse
NBS-SRM	National Bureau of Standards (now NIST)- Standard Reference Material
ND	no data <i>or</i> detection limit not determined
NEPA	National Environmental Policy Act
NF	not found in the sample matrix <i>or</i> not determined
NIST	National Institute of Science and Technology
nitro-PAH	nitropolycyclic aromatic hydrocarbons
NIOSH	National Institute for Occupational Safety and Health
NOSIH	Naval Ordnance Station, Indian Head, Maryland
NO _x	nitrogen oxides
NS	not sampled
OB	open burning
OB/OD	open burning/open detonation
OC	organic carbon
OD	open detonation
OGC	Oregon Graduate Center, Beaverton, Oregon
OSHA	Occupational Safety and Health Administration
PAH	polycyclic aromatic hydrocarbons
PANH	polycyclic aromatic nitrogen heterocycles
PAOH	polycyclic aromatic oxygen heterocycles
PCDD	polychlorinated dibenzodioxins
PCDF	polychlorinated dibenzofurans
PETN	pentaerythritol tetranitrate
PEP	propellants, explosives, and pyrotechnics
PIC	products of incomplete combustion
PICI/SIM	Positive ion chemical ionization/selective ion monitoring

PID	photoionization detector
PIP	product improvement program
PM	program manager
PMS	Particle Measuring Systems, Inc.
PUF	polyurethane foam
QA	quality assurance
QA/QC	quality assurance/quality control
QC	quality control
QAA	quality assurance agency
QAPP	quality assurance project plan
QAU	quality assurance unit
RCRA	Resource Conservation and Recovery Act
RDX	hexamethylenetrinitramine
RFD	Reno (Nevada) Fire Department
RIC	relative ion count
RSD	relative standard deviation
RTP	Research Triangle Park, North Carolina
SDPDA	Special Defense Property Disposal Account
SEM	scanning electron microscope/microscopy
SFC	supercritical fluid chromatography
SFC/MS	supercritical fluid chromatography/mass spectrometry
SF ₆	sulfur hexafluoride
SIM	selected-ion monitoring (or selective-ion monitoring)
SNL	Sandia National Laboratories, Albuquerque, New Mexico
SOP	standing operating procedures
SS	stainless steel
SSC	stainless steel canister
SSL	Sunset Laboratory, Forest Grove, Oregon
STEL	short-term exposure limit
STP	standard temperature and pressure (25°C and 760 torr)
TCD	thermal conductivity detector
TDP	test design plan

TEAD	U.S. Army Tooele Army Depot, Tooele, Utah
TECO	Thermo Electron Instruments (Company)
TECOM	U.S. Army Test and Evaluation Command, Aberdeen Proving Ground, Maryland
THC	total hydrocarbon
TLV	threshold limit values
TNT	2,4,6-trinitrotoluene
TSC	technical steering committee
TSP	total suspended particulate
TWA	time-weighted average
USATHAMA	U.S. Army Toxic and Hazardous Materials Agency, Aberdeen Proving Ground, Maryland
UV	ultraviolet
VOC	volatile organic compounds
VOST	semivolatile organic sampling train
VSDM	Volume Source Diffusion Model
XRF	X-ray fluorescence <i>or</i> X-ray fluorescence spectrometer

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APPENDIX J - GLOSSARY

B-48	The Sandia National Laboratories (SNL) mobile laboratory on-site at the U.S. Army Michael Army Airfield, Dugway Proving Ground, Utah. This laboratory contained filter support equipment and test equipment and parts for repairing instrumentation and sample collectors aboard the sampling aircraft.
BangBox	An inflatable 16-m diameter hemisphere used for conducting closed chamber tests involving detonation of small amounts of explosive and burning of small amounts of propellant.
burn pans	Steel pans used to contain propellants during burning and prevent soil contamination by residues.
cloud volume method	a procedure which uses carbon as a tracer for the products of a detonation or propellant burn in a cloud. Assumes that cloud of detonation or combustion products is homogeneous in relative composition. Volume of cloud is not required for computation of the mass of an analyte.
carbon balance method	a procedure which uses carbon as a tracer for the products of a detonation or propellant burn in a cloud. Assumes that cloud of detonation or combustion products is homogeneous in relative composition. Volume of cloud is not required for computation.
composition B	An explosive composed primarily of RDX and TNT in an approximately 60/40 ratio (by weight).
donor charge	A small explosive charge used to initiate the detonation of a substantially larger explosive charge. Sometimes referred to as an "initiator", "initiating charge", or "primer".

double-base propellant	A propellant consisting primarily of nitrocellulose and nitroglycerine. Mix used during OB/OD field test was approximately 50 percent nitrocellulose and 35 percent nitroglycerin.
ejecta	Soil displaced from the point of a surface detonation and which is deposited near the detonation crater.
exotics	Volatile organic compounds which, if detected during laboratory assay, would most likely be found at trace levels.
explosive D	An explosive consisting primarily of picric acid. Frequently referred to as "yellow D" due to its characteristic yellow color. Relatively insensitive and requires a substantially larger initiating charge than other military explosives to ensure complete detonation.
field test	A series of open-air trials using techniques and material identical to those used in, or proposed for, actual operations.
FWAC	A fixed-wing aircraft outfitted to sample, analyze, and collect combustion emissions from the open detonation of explosive and open burning of propellants.
Interim Test	A series of open-air trials using end-item PEP material which were conducted at the Tooele Army Depot during 1986.
kickout	Pieces of propellant ejected from burn pans either by low-level shock waves or thermal-generated drafts.
M1 Propellant	A single-base propellant used to fire projectiles by field artillery howitzers, and guns.
M6 Propellant	See M1 Propellant

Operational readiness inspection	A trial, frequently referred to as an "ORI", designed to ensure methods, equipments, and personnel are prepared to undertake subsequent data-gathering trials.
PBXN-6	Mixture of RDX and Viton A* in a 95/5 ratio. Referred to as "RDX" within this report.
PETN	A military explosive (pentaerythritol tetranitrate) commonly used in detonating cord.
propellant manufacturing residue	Incompletely manufactured propellant. No scrap material included in residue used during OB/OD field testing.
RDX	A military explosive consisting primarily of hexamethylenetrinitroamine. See PBXN-6.
single-base propellant	A propellant consisting of approximately 85 percent nitrocellulose.
sputter	Pieces of propellant ejected from burn pans by the energy of their burning.
sputter pan	A square metal pan designed and located so as to capture particles of propellants lofted out of burn pans during open burning testing.
supercritical fluid chromatography	SFC is a chromatographic technique where a supercritical fluid is used as the mobile phase. SFC has efficiencies comparable to that of gas chromatography and a solvating mobile phase such as in liquid chromatography.

surface detonation	A detonation which was set up with explosives set on the ground, or placed in a container set on the ground.
transport tube	The tube used to transport outside air into the FWAC for instrument sampling.
triple base propellant	A propellant consisting primarily of nitrocellulose, nitroglycerine, and nitroguanadine. Triple-base propellant used during OB/OD field testing was approximately 28 percent nitrocellulose, 22 percent nitroglycerin, and 48 percent nitroguanidine.
suspended detonation	A method used in the OB/OD Phase B and C tests to suspend 907 kg of TNT in steel drums 40 feet off the ground for subsequent detonation.
TNT	An explosive consisting almost exclusively of trinitrotoluene.
washout explosive	Explosive reclaimed from munitions by a process of opening a munition and removing the explosive filler by flushing the casing/container with high-pressure hot water.
yellow D	See explosive D.

APPENDIX K - OB/OD PROGRAM SYNOPSIS

1. Original Study Purpose

The original OB/OD study was intended to provide munitions and propellant thermal treatment emissions data to satisfy increasingly stringent state and Federal permitting requirements.

2. Interim Test

The initial effort, now referred to as the Interim Test, was conducted at the Tooele Army Depot with the objective of directly obtaining this data. End-item munitions and propellants were tested, and a variety of samplers, real-time analyzers, and assay procedures used to characterize their combustion products. This test did not meet its objectives because the technology to detect and quantify emissions at desired levels had either not been developed, or was not made available to the project.

3. Program Reevaluation

Upon conclusion of the Interim Test and after consultation with certain EPA agencies, the decision was made that an orderly, scientific methodology was necessary to provide accurate and replicable test data which would satisfy current and anticipated requirements of state and Federal environmental regulatory agencies. This would necessarily involve use of state-of-the-art technologies and instruments capable of meeting anticipated regulatory agency requirements.

4. Current OB/OD Phase

4.1 Objectives

4.1.1 The recently-concluded phase of the OB/OD Thermal Treatment Emissions Study was designed and conducted as the first step of this premise, i.e., to find, test, and authenticate technologies and procedures which could then be used to obtain data to support OB/OD permitting. An ancillary objective was to ascertain if small-scale controlled testing could be related to large-scale

field testing and thus reduce the time and expense which typify large-scale testing.

4.1.2 The types of bulk explosives and propellants tested are components of a large percentage of demilitarization account end items. Munition-specific variables such as shell-casing components were not tested; however, with high-order detonation of complete munitions, the same combustion products are expected.

4.2 Results

4.2.1 The primary consequence of this testing was the assessment of instruments' and procedures' abilities to accurately capture and analyze combustion products, and the evaluation of scaling BB data to field data for detonations and burns. The secondary consequence was characterization of emission products imparted into the atmosphere and soil for the items tested.

4.2.2 The emission data along with meteorological diffusion models can generate expected downwind dosage values which can be compared with ambient air concentration limits set by states. The ejecta concentration data for the soil in the crater area can be used to estimate the total amount of the analyte that remains in the soil after a detonation. Fallout concentrations can be used to determine the analyte and the amount that is deposited on the undisturbed surface.

4.2.3 Results of the small-scale BangBox and large-scale field tests are highly encouraging. Both procedures and instruments were proved to be accurate and capable of meeting the requirements of the study. The amount of pollutants released into the atmosphere and soil were considered inconsequential.

4.2.4 The data indicates that, for those items tested, there is no serious impact to the environment; however, further studies must be done to determine the full environmental impact of OB/OD thermal treatment methods for the following reasons:

4.2.4.1 Bulk explosives constitute only a small fraction of the demilitarization inventory.

4.2.4.2 Their combustion products may not represent combustion products of encased munitions

4.2.4.3 Tests were site-specific only to a single locale.

4.2.4.4 The procedures used did not represent procedures customarily used at some treatment facilities, e.g. buried detonations.

4.3 Status

4.3.1 The current phase of the OB/OD study authenticated acceptable technology and methodology that can be used to obtain the munition- and site-specific emission characterization data. This data may then be used as part of the information needed to obtain permits for continued OB/OD operations. The data can be acquired by either constructing a single BangBox at a single site or constructing a BangBox at each specific site for emission characterization of site-specific munitions and soil.

4.3.2 An OB/OD dispersion model was also developed during the field trials of the study. A model acceptable to EPA is an essential adjunct to the BangBox emission characterization data in that it provides the mechanism to generate downwind concentrations at receptor locations, and input required for risk assessment to support site-specific permit applications. The model will require refinement and field validation before being made available to potential users.

4.3.3 As site- and munition-specific emissions data are collected and evaluated, they can provide part of the basis for risk assessment input which will evaluate which munitions, and explosive and propellants in the DoD inventory are applicable to OB/OD treatment, and which are not. For those not appropriate, the emissions characterization data can be used to more effectively focus efforts on the development and permitting of required alternative technologies.

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